Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 02:45 am GMT

PDB ID	:	8OOO
Title	:	Glutamine synthetase from Methanothermococcus thermolithotrophicus in complex with 2-oxoglutarate and MgATP at 2.15 A resolution
Authors	:	Mueller, M.-C.; Wagner, T.
Deposited on	:	2023-04-05
Resolution	:	2.15 Å(reported)

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

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

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

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

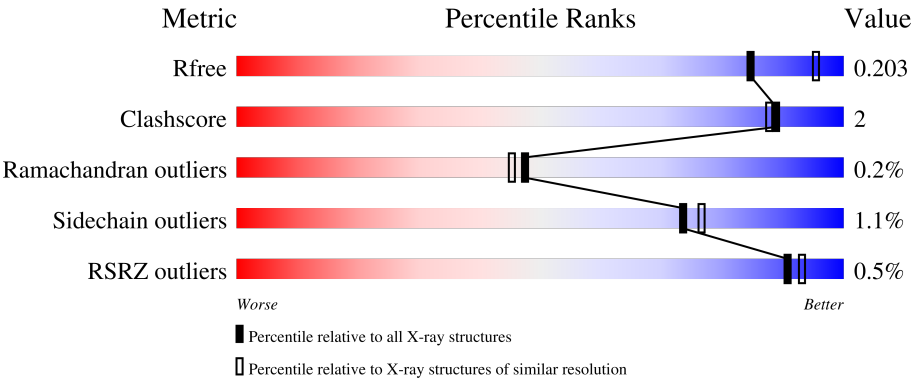
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	448	95% 5%
1	B	448	96% .
1	C	448	96% .
1	D	448	93% 6%
1	E	448	% 95% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	448	95%
1	G	448	94% 6%
1	H	448	95%
1	I	448	95% 5%
1	J	448	96%
1	K	448	96%
1	L	448	94% 5%

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
3	PEG	K	501	-	-	X	-

2 Entry composition (i)

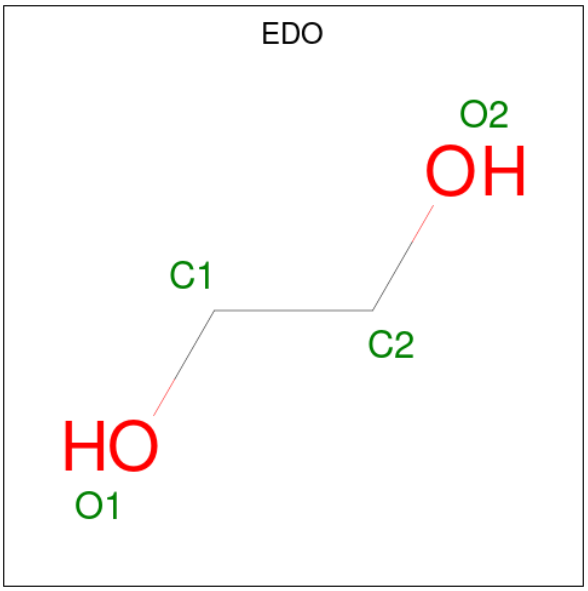
There are 10 unique types of molecules in this entry. The entry contains 46159 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase from Methanothermococcus thermolithotrophicus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	B	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	C	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	D	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	E	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	F	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	G	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	H	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	I	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	J	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	K	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			
1	L	447	Total	C	N	O	S	0	0	0
			3534	2264	587	667	16			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



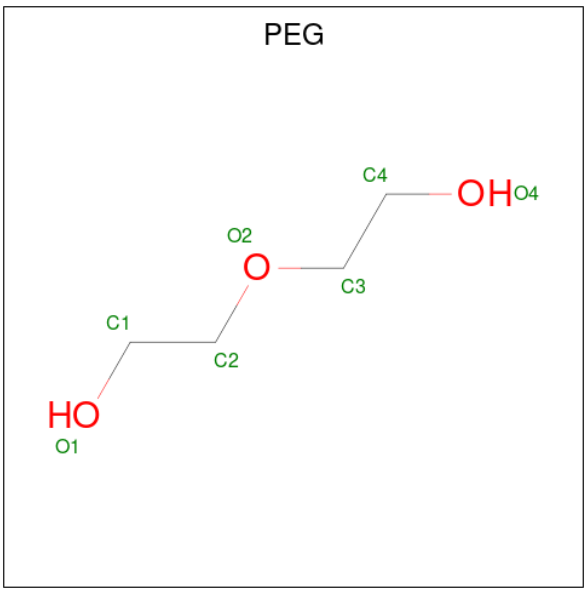
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total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

Continued on next page...

Continued from previous page...

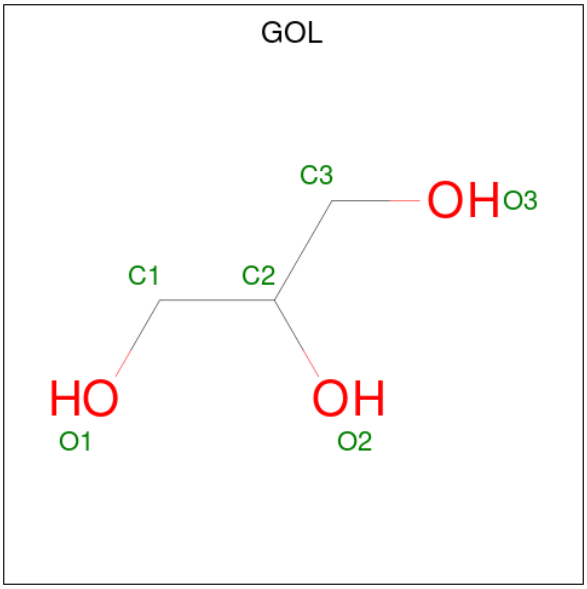
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	G	1	Total C O 7 4 3	0	0
3	G	1	Total C O 6 4 2	0	0
3	G	1	Total C O 7 4 3	0	0
3	G	1	Total C O 7 4 3	0	0
3	J	1	Total C O 7 4 3	0	0
3	K	1	Total C O 7 4 3	0	0

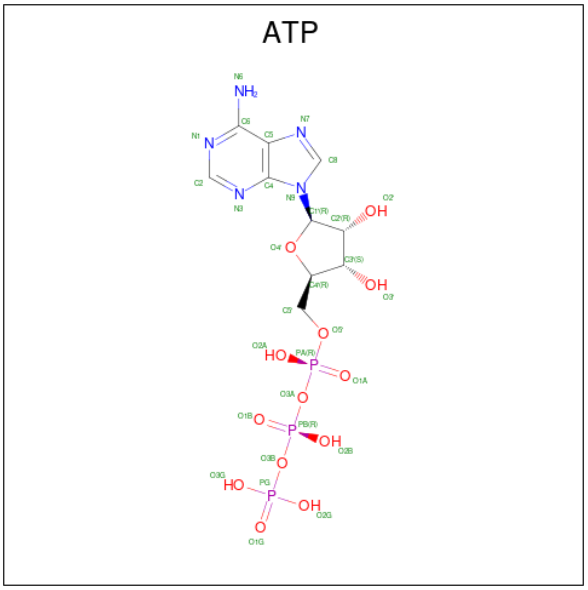
- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

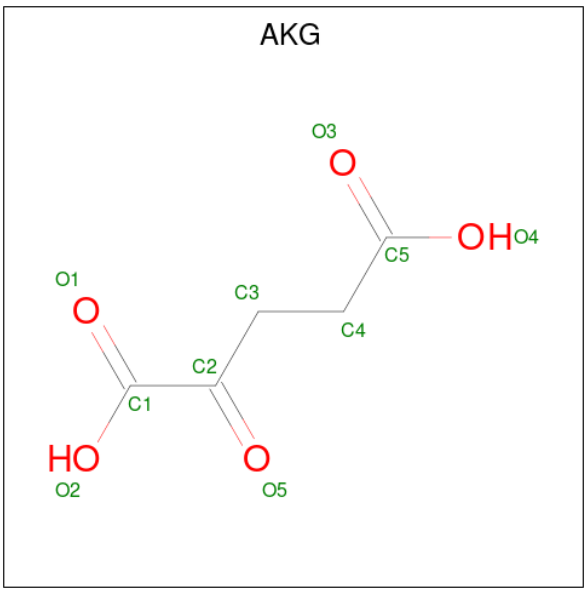
$C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	I	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	J	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	K	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	L	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

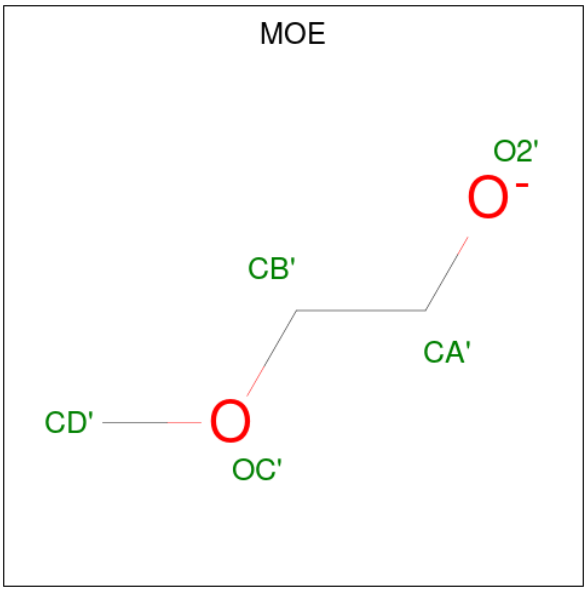
- Molecule 6 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$) (la-

beled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 10 5 5	0	0
6	B	1	Total C O 10 5 5	0	0
6	C	1	Total C O 10 5 5	0	0
6	D	1	Total C O 10 5 5	0	0
6	E	1	Total C O 10 5 5	0	0
6	F	1	Total C O 10 5 5	0	0
6	G	1	Total C O 10 5 5	0	0
6	H	1	Total C O 10 5 5	0	0
6	I	1	Total C O 10 5 5	0	0
6	J	1	Total C O 10 5 5	0	0
6	K	1	Total C O 10 5 5	0	0
6	L	1	Total C O 10 5 5	0	0

- Molecule 7 is METHOXY-ETHOXYL (three-letter code: MOE) (formula: $C_3H_7O_2$).

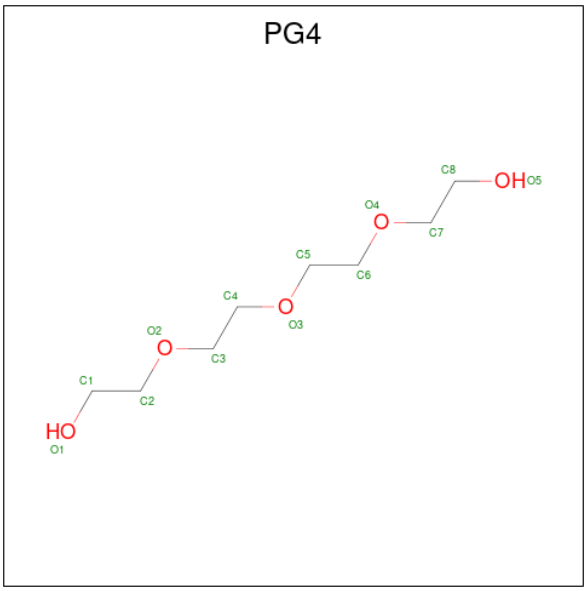


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 5 3 2	0	0
7	F	1	Total C O 5 3 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Mg 1 1	0	0
8	E	1	Total Mg 1 1	0	0
8	K	1	Total Mg 1 1	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 13 8 5	0	0
9	D	1	Total C O 13 8 5	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	249	Total O 249 249	0	0
10	B	219	Total O 219 219	0	0
10	C	257	Total O 257 257	0	0
10	D	260	Total O 260 260	0	0
10	E	242	Total O 242 242	0	0
10	F	274	Total O 274 274	0	0
10	G	265	Total O 265 265	0	0
10	H	251	Total O 251 251	0	0
10	I	250	Total O 250 250	0	0
10	J	249	Total O 249 249	0	0

Continued on next page...

Continued from previous page...

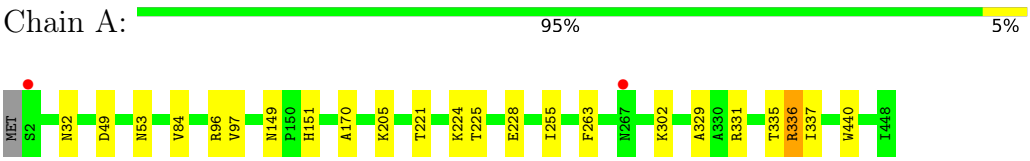
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	K	267	Total O 267 267	0	0
10	L	258	Total O 258 258	0	0

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.

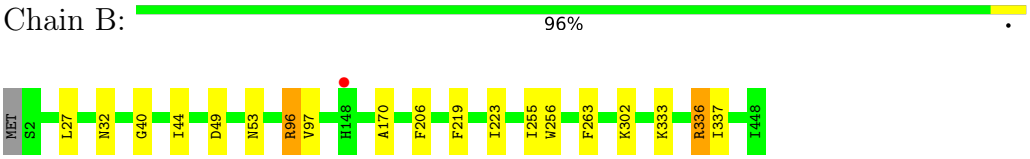
• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain A:



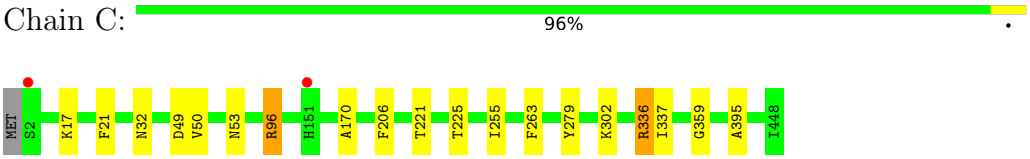
• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain B:



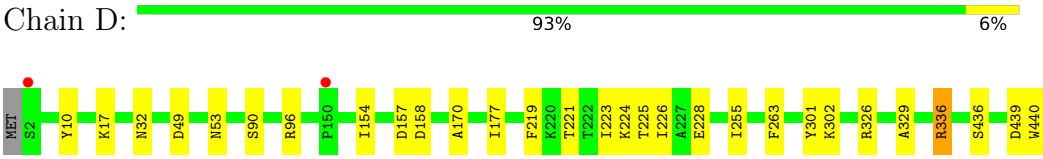
• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain C:



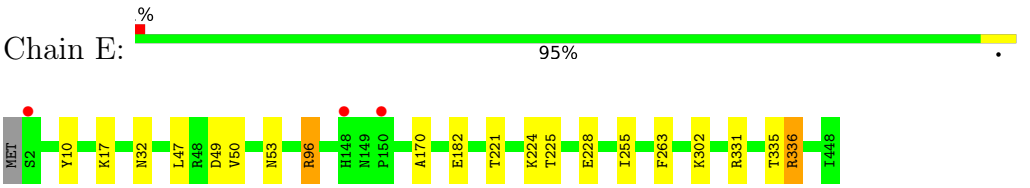
• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain D:



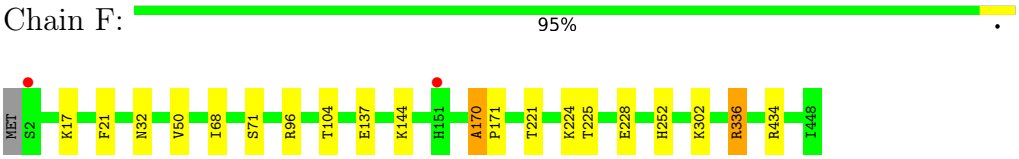
• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain E:



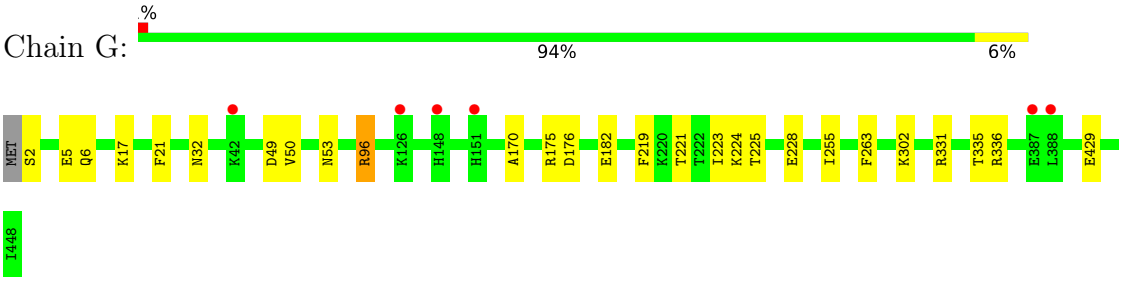
• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain F:



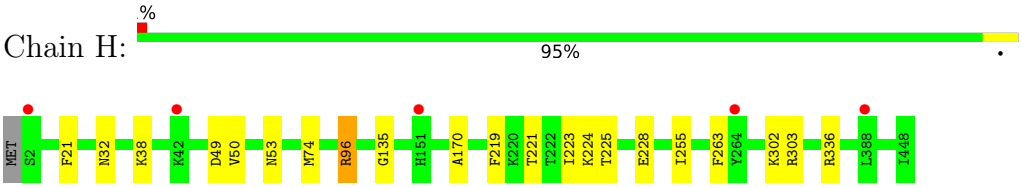
• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain G:



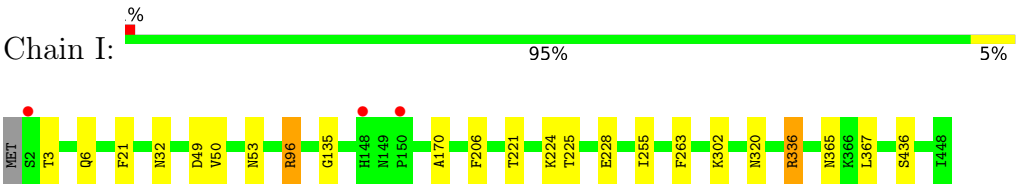
• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain H:



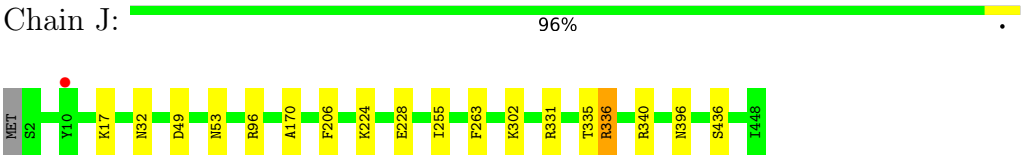
• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain I:



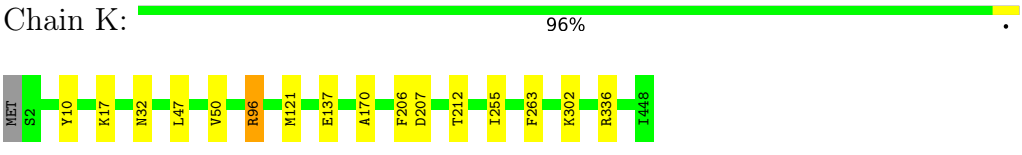
• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain J:



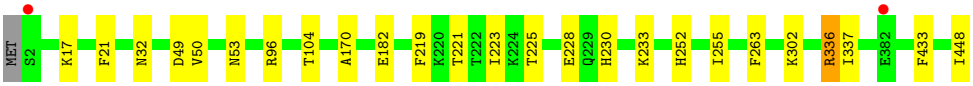
• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain K:



• Molecule 1: Glutamine synthetase from Methanothermococcus thermolithotrophicus

Chain L:


MET
S2
K17
F21
N32
D49
V50
N53
R96
T104
A170
E182
F219
K220
T221
T222
I223
K224
T225
E228
Q229
H230
K233
H252
I255
F263
K302
R336
I337
E382
F433
I448

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	112.34Å 131.77Å 131.51Å 60.04° 87.72° 67.34°	Depositor
Resolution (Å)	42.88 – 2.15 111.84 – 2.15	Depositor EDS
% Data completeness (in resolution range)	77.0 (42.88-2.15) 76.9 (111.84-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.14Å)	Xtriage
Refinement program	BUSTER 2.10.4 (21-NOV-2022)	Depositor
R, R_{free}	0.182 , 0.214 0.171 , 0.203	Depositor DCC
R_{free} test set	12085 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.064 for -h,-k+l,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	46159	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: MG, PEG, AKG, PG4, EDO, MOE, ATP, GOL

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	0.47	0/3625	0.55	0/4910
1	B	0.46	0/3625	0.55	0/4910
1	C	0.45	0/3625	0.55	0/4910
1	D	0.46	0/3625	0.55	0/4910
1	E	0.46	0/3625	0.55	0/4910
1	F	0.47	0/3625	0.56	0/4910
1	G	0.46	0/3625	0.55	0/4910
1	H	0.45	0/3625	0.54	0/4910
1	I	0.44	0/3625	0.55	0/4910
1	J	0.48	0/3625	0.55	0/4910
1	K	0.46	0/3625	0.56	0/4910
1	L	0.47	0/3625	0.55	0/4910
All	All	0.46	0/43500	0.55	0/58920

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3534	0	3458	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3534	0	3458	11	0
1	C	3534	0	3458	11	0
1	D	3534	0	3458	21	0
1	E	3534	0	3458	12	0
1	F	3534	0	3458	12	0
1	G	3534	0	3458	15	0
1	H	3534	0	3458	12	0
1	I	3534	0	3458	13	0
1	J	3534	0	3458	10	0
1	K	3534	0	3458	14	0
1	L	3534	0	3458	18	0
2	A	16	0	24	2	0
2	B	12	0	18	0	0
2	C	12	0	18	2	0
2	D	4	0	6	1	0
2	E	4	0	6	0	0
2	F	16	0	24	2	0
2	G	4	0	6	0	0
2	H	4	0	6	1	0
2	I	12	0	18	1	0
2	J	8	0	12	1	0
2	L	12	0	18	0	0
3	A	14	0	20	1	0
3	D	14	0	20	4	0
3	G	27	0	37	6	0
3	J	7	0	10	1	0
3	K	7	0	10	4	0
4	A	6	0	8	1	0
5	A	31	0	12	1	0
5	B	31	0	12	2	0
5	C	31	0	12	2	0
5	D	31	0	12	2	0
5	E	31	0	12	1	0
5	F	31	0	12	1	0
5	G	31	0	12	0	0
5	H	31	0	12	2	0
5	I	31	0	12	3	0
5	J	31	0	12	2	0
5	K	31	0	12	2	0
5	L	31	0	12	2	0
6	A	10	0	4	0	0
6	B	10	0	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	10	0	4	0	0
6	D	10	0	4	0	0
6	E	10	0	4	0	0
6	F	10	0	4	0	0
6	G	10	0	4	0	0
6	H	10	0	4	0	0
6	I	10	0	4	0	0
6	J	10	0	4	0	0
6	K	10	0	4	0	0
6	L	10	0	4	0	0
7	B	5	0	7	1	0
7	F	5	0	7	0	0
8	B	1	0	0	0	0
8	E	1	0	0	0	0
8	K	1	0	0	0	0
9	D	26	0	36	8	0
10	A	249	0	0	0	0
10	B	219	0	0	1	0
10	C	257	0	0	0	0
10	D	260	0	0	0	0
10	E	242	0	0	2	0
10	F	274	0	0	0	0
10	G	265	0	0	1	0
10	H	251	0	0	1	0
10	I	250	0	0	1	0
10	J	249	0	0	0	0
10	K	267	0	0	1	0
10	L	258	0	0	2	0
All	All	46159	0	41999	161	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 2.

All (161) 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:G:2:SER:HB3	1:G:5:GLU:HB2	1.75	0.67
1:I:336:ARG:HD2	5:I:504:ATP:C5	2.34	0.63
1:D:336:ARG:HD2	5:D:506:ATP:C5	2.36	0.61
1:J:436:SER:HB2	3:J:801:PEG:H12	1.83	0.61
1:D:326:ARG:NH2	5:D:506:ATP:O1B	2.25	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:340:ARG:HH21	2:J:803:EDO:H12	1.67	0.58
1:F:137:GLU:OE2	5:F:506:ATP:O2G	2.22	0.58
3:G:603:PEG:H32	1:L:448:ILE:HG21	1.85	0.57
1:D:443:THR:HB	9:D:501:PG4:H32	1.85	0.57
1:B:337:ILE:HG13	1:B:337:ILE:O	2.04	0.57
1:D:154:ILE:HD12	3:D:504:PEG:H41	1.87	0.57
1:D:177:ILE:HG13	1:D:226:ILE:HG21	1.88	0.55
1:A:336:ARG:HD2	5:A:508:ATP:C5	2.42	0.55
2:A:501:EDO:H12	10:E:798:HOH:O	2.07	0.55
1:F:17:LYS:O	1:F:17:LYS:HD3	2.07	0.55
1:G:224:LYS:O	1:G:228:GLU:HG2	2.06	0.55
1:L:233:LYS:NZ	10:L:601:HOH:O	2.31	0.55
1:E:96:ARG:HD2	1:E:96:ARG:C	2.28	0.54
1:E:336:ARG:HD2	5:E:604:ATP:C5	2.41	0.54
1:C:337:ILE:O	1:C:337:ILE:HG13	2.06	0.54
3:G:603:PEG:H22	10:G:854:HOH:O	2.07	0.54
1:A:205:LYS:HD3	3:A:504:PEG:H32	1.90	0.54
1:G:17:LYS:O	1:G:17:LYS:HD3	2.08	0.54
1:D:443:THR:CG2	9:D:501:PG4:H32	2.38	0.53
1:H:135:GLY:HA3	5:H:603:ATP:H1'	1.89	0.53
1:E:182:GLU:HG2	10:E:791:HOH:O	2.09	0.53
1:K:212:THR:OG1	3:K:501:PEG:H41	2.08	0.53
1:D:17:LYS:O	1:D:17:LYS:HD3	2.08	0.53
1:L:21:PHE:CZ	1:L:50:VAL:HG12	2.44	0.53
1:L:17:LYS:HD3	1:L:17:LYS:O	2.09	0.52
1:G:96:ARG:HD2	1:G:96:ARG:C	2.30	0.52
1:K:47:LEU:HA	1:K:50:VAL:HG22	1.92	0.52
1:L:252:HIS:CE1	5:L:505:ATP:H5'1	2.44	0.51
1:J:17:LYS:O	1:J:17:LYS:HD3	2.11	0.51
1:B:96:ARG:HD2	1:B:96:ARG:C	2.31	0.51
1:C:17:LYS:O	1:C:17:LYS:HD3	2.10	0.51
1:C:336:ARG:HD2	5:C:604:ATP:C5	2.45	0.50
1:L:337:ILE:O	1:L:337:ILE:HG13	2.12	0.50
1:L:230:HIS:HD2	10:L:837:HOH:O	1.93	0.50
1:B:219:PHE:O	1:B:223:ILE:HD13	2.12	0.50
1:D:440:TRP:HA	9:D:501:PG4:H52	1.93	0.50
9:D:505:PG4:H11	1:J:396:ASN:HB3	1.93	0.50
1:C:206:PHE:HB3	5:C:604:ATP:H1'	1.93	0.49
1:L:252:HIS:HB3	1:L:336:ARG:HG3	1.94	0.49
1:A:49:ASP:OD1	1:A:53:ASN:ND2	2.46	0.49
1:K:137:GLU:OE2	5:K:504:ATP:O2G	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:ASP:OD1	3:D:504:PEG:H32	2.13	0.49
1:C:279:TYR:CE1	1:C:359:GLY:HA3	2.48	0.48
1:B:27:LEU:HB3	7:B:503:MOE:HD'2	1.96	0.48
1:G:331:ARG:HA	1:G:335:THR:OG1	2.14	0.48
1:H:336:ARG:HD2	5:H:603:ATP:C5	2.49	0.48
1:A:84:VAL:HG23	4:A:507:GOL:H11	1.95	0.48
1:B:336:ARG:HD2	5:B:506:ATP:C5	2.49	0.48
1:H:21:PHE:CZ	1:H:50:VAL:HG12	2.49	0.47
1:D:439:ASP:HB2	9:D:501:PG4:H81	1.95	0.47
1:E:17:LYS:O	1:E:17:LYS:HD3	2.14	0.47
1:J:206:PHE:HB3	5:J:805:ATP:H1'	1.97	0.47
1:E:224:LYS:O	1:E:228:GLU:HG2	2.15	0.47
1:G:21:PHE:CZ	1:G:50:VAL:HG12	2.49	0.47
1:G:175:ARG:HH21	3:G:601:PEG:H12	1.80	0.47
1:K:207:ASP:HB2	3:K:501:PEG:C4	2.45	0.47
1:D:219:PHE:O	1:D:223:ILE:HD13	2.14	0.47
1:F:252:HIS:HB3	1:F:336:ARG:HG3	1.97	0.47
1:D:224:LYS:O	1:D:228:GLU:HG2	2.15	0.47
1:H:303:ARG:HE	2:H:601:EDO:H21	1.79	0.46
1:K:206:PHE:HB3	5:K:504:ATP:H1'	1.97	0.46
1:B:256:TRP:HH2	1:B:333:LYS:HG2	1.81	0.46
1:A:224:LYS:O	1:A:228:GLU:HG2	2.15	0.46
1:F:224:LYS:O	1:F:228:GLU:HG2	2.16	0.46
1:J:336:ARG:HD2	5:J:805:ATP:C5	2.51	0.46
1:C:21:PHE:CZ	1:C:50:VAL:HG12	2.50	0.46
1:H:74:MET:HE1	10:H:738:HOH:O	2.15	0.46
1:C:96:ARG:HD2	1:C:96:ARG:C	2.35	0.45
1:D:221:THR:O	1:D:225:THR:HG23	2.16	0.45
1:F:68:ILE:O	1:F:71:SER:OG	2.28	0.45
3:D:503:PEG:H11	3:D:503:PEG:H32	1.50	0.45
1:K:96:ARG:HD2	1:K:96:ARG:C	2.36	0.45
1:D:49:ASP:OD1	1:D:53:ASN:ND2	2.50	0.45
1:G:2:SER:O	1:G:6:GLN:HG3	2.16	0.45
1:I:320:ASN:HB2	10:I:642:HOH:O	2.17	0.45
1:F:21:PHE:CZ	1:F:50:VAL:HG12	2.51	0.45
1:A:440:TRP:HA	2:A:501:EDO:H22	1.99	0.45
1:D:329:ALA:HB1	1:F:104:THR:HG21	1.99	0.45
1:G:176:ASP:OD1	3:G:601:PEG:H32	2.17	0.45
1:J:331:ARG:HA	1:J:335:THR:OG1	2.17	0.45
1:A:221:THR:O	1:A:225:THR:HG23	2.16	0.44
1:K:17:LYS:NZ	1:L:182:GLU:OE2	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:501:PG4:H41	9:D:501:PG4:H22	1.78	0.44
1:H:96:ARG:HD2	1:H:96:ARG:C	2.38	0.44
1:K:10:TYR:CD1	1:K:10:TYR:C	2.91	0.44
1:L:49:ASP:OD1	1:L:53:ASN:ND2	2.51	0.44
1:E:49:ASP:OD1	1:E:53:ASN:ND2	2.49	0.44
1:I:49:ASP:OD1	1:I:53:ASN:ND2	2.50	0.44
1:I:21:PHE:CZ	1:I:50:VAL:HG12	2.52	0.44
1:I:221:THR:O	1:I:225:THR:HG23	2.18	0.43
1:F:221:THR:O	1:F:225:THR:HG23	2.18	0.43
1:A:331:ARG:HA	1:A:335:THR:OG1	2.17	0.43
1:E:331:ARG:HA	1:E:335:THR:OG1	2.18	0.43
1:I:135:GLY:HA3	5:I:504:ATP:H1'	2.00	0.43
1:J:224:LYS:O	1:J:228:GLU:HG2	2.19	0.43
1:B:255:ILE:HG12	1:B:263:PHE:CE1	2.54	0.43
1:B:40:GLY:O	1:B:44:ILE:HG12	2.19	0.43
1:F:144:LYS:HZ3	2:F:503:EDO:H12	1.83	0.43
1:H:219:PHE:O	1:H:223:ILE:HD13	2.18	0.43
1:K:207:ASP:HB2	3:K:501:PEG:H42	2.01	0.43
1:F:144:LYS:NZ	2:F:503:EDO:H12	2.33	0.43
1:B:97:VAL:HG13	1:B:97:VAL:O	2.17	0.43
1:I:3:THR:HG22	1:I:6:GLN:OE1	2.18	0.43
1:E:17:LYS:NZ	1:G:182:GLU:OE2	2.52	0.43
1:G:49:ASP:OD1	1:G:53:ASN:ND2	2.52	0.43
1:I:255:ILE:HG12	1:I:263:PHE:CE1	2.54	0.43
1:D:157:ASP:HA	3:D:504:PEG:H12	2.00	0.42
1:G:429:GLU:HG3	3:G:602:PEG:H22	2.00	0.42
1:J:49:ASP:OD1	1:J:53:ASN:ND2	2.52	0.42
1:J:255:ILE:HG12	1:J:263:PHE:CE1	2.54	0.42
1:C:395:ALA:CB	2:C:603:EDO:H11	2.48	0.42
1:D:255:ILE:HG12	1:D:263:PHE:CE1	2.54	0.42
1:E:10:TYR:C	1:E:10:TYR:CD1	2.91	0.42
1:A:337:ILE:O	1:A:337:ILE:HG13	2.20	0.42
1:H:49:ASP:OD1	1:H:53:ASN:ND2	2.52	0.42
1:H:224:LYS:O	1:H:228:GLU:HG2	2.19	0.42
1:A:329:ALA:HB1	1:L:104:THR:HG21	2.01	0.42
1:D:436:SER:HB2	2:D:502:EDO:H11	2.02	0.42
1:F:170:ALA:N	1:F:171:PRO:HD3	2.34	0.42
1:G:219:PHE:O	1:G:223:ILE:HD13	2.19	0.42
1:G:255:ILE:HG12	1:G:263:PHE:CE1	2.55	0.42
1:K:121:MET:HE2	10:K:679:HOH:O	2.20	0.42
2:C:603:EDO:H12	1:F:434:ARG:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:LYS:O	1:I:228:GLU:HG2	2.19	0.41
1:L:221:THR:O	1:L:225:THR:HG23	2.20	0.41
1:C:221:THR:O	1:C:225:THR:HG23	2.19	0.41
1:D:443:THR:CB	9:D:501:PG4:H32	2.49	0.41
1:E:255:ILE:HG12	1:E:263:PHE:CE1	2.56	0.41
1:B:49:ASP:OD1	1:B:53:ASN:ND2	2.54	0.41
1:L:255:ILE:HG12	1:L:263:PHE:CE1	2.54	0.41
1:C:255:ILE:HG12	1:C:263:PHE:CE1	2.55	0.41
1:L:336:ARG:HD2	5:L:505:ATP:C5	2.54	0.41
1:D:301:TYR:HB2	9:D:505:PG4:C8	2.51	0.41
1:K:17:LYS:O	1:K:17:LYS:HD3	2.20	0.41
1:A:255:ILE:HG12	1:A:263:PHE:CE1	2.55	0.41
10:B:676:HOH:O	1:H:38:LYS:HE3	2.20	0.41
1:I:365:ASN:HB2	1:I:367:LEU:HD13	2.03	0.41
1:K:47:LEU:HA	1:K:50:VAL:CG2	2.50	0.41
1:C:49:ASP:OD1	1:C:53:ASN:ND2	2.52	0.41
1:E:221:THR:O	1:E:225:THR:HG23	2.20	0.41
1:G:221:THR:O	1:G:225:THR:HG23	2.21	0.41
1:K:207:ASP:CB	3:K:501:PEG:H41	2.51	0.41
1:E:47:LEU:HA	1:E:50:VAL:HG22	2.02	0.41
1:I:436:SER:HB2	2:I:501:EDO:H12	2.03	0.41
1:L:219:PHE:O	1:L:223:ILE:HD13	2.21	0.41
1:D:10:TYR:CD1	1:D:10:TYR:C	2.95	0.41
1:H:221:THR:O	1:H:225:THR:HG23	2.21	0.41
1:I:206:PHE:HB3	5:I:504:ATP:H1'	2.03	0.41
3:G:604:PEG:H31	1:L:433:PHE:HE2	1.85	0.40
1:L:219:PHE:O	1:L:223:ILE:CD1	2.69	0.40
1:L:228:GLU:OE2	1:L:228:GLU:HA	2.21	0.40
1:H:255:ILE:HG12	1:H:263:PHE:CE1	2.56	0.40
1:A:149:ASN:OD1	1:A:151:HIS:HB2	2.21	0.40
1:B:206:PHE:HB3	5:B:506:ATP:H1'	2.03	0.40
1:I:96:ARG:C	1:I:96:ARG:HD2	2.41	0.40
1:K:255:ILE:HG12	1:K:263:PHE:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	47	45
1	B	445/448 (99%)	437 (98%)	7 (2%)	1 (0%)	47	45
1	C	445/448 (99%)	437 (98%)	7 (2%)	1 (0%)	47	45
1	D	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	47	45
1	E	445/448 (99%)	435 (98%)	9 (2%)	1 (0%)	47	45
1	F	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	47	45
1	G	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	47	45
1	H	445/448 (99%)	435 (98%)	9 (2%)	1 (0%)	47	45
1	I	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	47	45
1	J	445/448 (99%)	436 (98%)	8 (2%)	1 (0%)	47	45
1	K	445/448 (99%)	434 (98%)	10 (2%)	1 (0%)	47	45
1	L	445/448 (99%)	435 (98%)	9 (2%)	1 (0%)	47	45
All	All	5340/5376 (99%)	5229 (98%)	99 (2%)	12 (0%)	47	45

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	ALA
1	E	170	ALA
1	H	170	ALA
1	A	170	ALA
1	C	170	ALA
1	D	170	ALA
1	F	170	ALA
1	G	170	ALA
1	I	170	ALA
1	J	170	ALA
1	K	170	ALA
1	L	170	ALA

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	382/383 (100%)	377 (99%)	5 (1%)	69	73
1	B	382/383 (100%)	378 (99%)	4 (1%)	76	79
1	C	382/383 (100%)	378 (99%)	4 (1%)	76	79
1	D	382/383 (100%)	377 (99%)	5 (1%)	69	73
1	E	382/383 (100%)	378 (99%)	4 (1%)	76	79
1	F	382/383 (100%)	378 (99%)	4 (1%)	76	79
1	G	382/383 (100%)	378 (99%)	4 (1%)	76	79
1	H	382/383 (100%)	379 (99%)	3 (1%)	81	85
1	I	382/383 (100%)	378 (99%)	4 (1%)	76	79
1	J	382/383 (100%)	378 (99%)	4 (1%)	76	79
1	K	382/383 (100%)	378 (99%)	4 (1%)	76	79
1	L	382/383 (100%)	378 (99%)	4 (1%)	76	79
All	All	4584/4596 (100%)	4535 (99%)	49 (1%)	73	76

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	96	ARG
1	A	97	VAL
1	A	302	LYS
1	A	336	ARG
1	B	32	ASN
1	B	96	ARG
1	B	302	LYS
1	B	336	ARG
1	C	32	ASN
1	C	96	ARG
1	C	302	LYS
1	C	336	ARG
1	D	32	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	90	SER
1	D	96	ARG
1	D	302	LYS
1	D	336	ARG
1	E	32	ASN
1	E	96	ARG
1	E	302	LYS
1	E	336	ARG
1	F	32	ASN
1	F	96	ARG
1	F	302	LYS
1	F	336	ARG
1	G	32	ASN
1	G	96	ARG
1	G	302	LYS
1	G	336	ARG
1	H	32	ASN
1	H	96	ARG
1	H	302	LYS
1	I	32	ASN
1	I	96	ARG
1	I	302	LYS
1	I	336	ARG
1	J	32	ASN
1	J	96	ARG
1	J	302	LYS
1	J	336	ARG
1	K	32	ASN
1	K	96	ARG
1	K	302	LYS
1	K	336	ARG
1	L	32	ASN
1	L	96	ARG
1	L	302	LYS
1	L	336	ARG

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

Mol	Chain	Res	Type
1	A	14	ASN
1	F	278	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 68 ligands modelled in this entry, 3 are monoatomic - leaving 65 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	J	802	-	3,3,3	0.17	0	2,2,2	0.20	0
5	ATP	J	805	-	26,33,33	0.88	1 (3%)	31,52,52	1.36	7 (22%)
5	ATP	L	505	-	26,33,33	0.91	1 (3%)	31,52,52	1.35	6 (19%)
5	ATP	E	604	8	26,33,33	0.88	1 (3%)	31,52,52	1.39	6 (19%)
2	EDO	B	501	-	3,3,3	0.39	0	2,2,2	0.35	0
3	PEG	A	502	-	6,6,6	0.09	0	5,5,5	0.06	0
6	AKG	B	507	-	9,9,9	1.70	1 (11%)	11,11,11	1.42	2 (18%)
2	EDO	A	505	-	3,3,3	0.13	0	2,2,2	0.18	0
3	PEG	A	504	-	6,6,6	0.11	0	5,5,5	0.07	0
2	EDO	A	503	-	3,3,3	0.15	0	2,2,2	0.19	0
5	ATP	D	506	-	26,33,33	0.90	1 (3%)	31,52,52	1.37	5 (16%)
2	EDO	F	503	-	3,3,3	0.15	0	2,2,2	0.22	0
2	EDO	I	505	-	3,3,3	0.76	0	2,2,2	0.36	0
6	AKG	F	505	-	9,9,9	2.03	2 (22%)	11,11,11	1.05	0
2	EDO	J	803	-	3,3,3	0.17	0	2,2,2	0.20	0
6	AKG	E	603	-	9,9,9	2.49	2 (22%)	11,11,11	1.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	AKG	G	606	-	9,9,9	1.83	1 (11%)	11,11,11	1.61	3 (27%)
2	EDO	F	501	-	3,3,3	0.64	0	2,2,2	0.13	0
7	MOE	B	503	-	4,4,4	0.21	0	3,3,3	0.19	0
2	EDO	I	501	-	3,3,3	0.16	0	2,2,2	0.18	0
3	PEG	G	601	-	6,6,6	0.12	0	5,5,5	0.09	0
2	EDO	L	501	-	3,3,3	0.18	0	2,2,2	0.20	0
3	PEG	G	603	-	6,6,6	0.12	0	5,5,5	0.08	0
5	ATP	G	607	-	26,33,33	0.89	1 (3%)	31,52,52	1.33	4 (12%)
6	AKG	A	509	-	9,9,9	2.08	1 (11%)	11,11,11	1.83	2 (18%)
3	PEG	D	503	-	6,6,6	0.12	0	5,5,5	0.09	0
2	EDO	D	502	-	3,3,3	0.17	0	2,2,2	0.20	0
5	ATP	C	604	-	26,33,33	0.86	1 (3%)	31,52,52	1.39	5 (16%)
6	AKG	J	804	-	9,9,9	1.97	1 (11%)	11,11,11	1.35	1 (9%)
2	EDO	F	502	-	3,3,3	0.69	0	2,2,2	0.36	0
2	EDO	F	504	-	3,3,3	0.17	0	2,2,2	0.20	0
3	PEG	D	504	-	6,6,6	0.11	0	5,5,5	0.07	0
3	PEG	G	604	-	6,6,6	0.14	0	5,5,5	0.12	0
6	AKG	I	503	-	9,9,9	1.84	1 (11%)	11,11,11	1.06	0
5	ATP	H	603	-	26,33,33	0.89	1 (3%)	31,52,52	1.35	4 (12%)
2	EDO	B	502	-	3,3,3	0.21	0	2,2,2	0.19	0
9	PG4	D	501	-	12,12,12	0.15	0	11,11,11	0.17	0
4	GOL	A	507	-	5,5,5	0.09	0	5,5,5	0.34	0
2	EDO	L	502	-	3,3,3	0.14	0	2,2,2	0.20	0
6	AKG	C	605	-	9,9,9	2.42	1 (11%)	11,11,11	1.21	0
3	PEG	K	501	-	6,6,6	0.11	0	5,5,5	0.08	0
2	EDO	C	602	-	3,3,3	0.18	0	2,2,2	0.27	0
7	MOE	F	507	-	4,4,4	0.20	0	3,3,3	0.21	0
2	EDO	A	501	-	3,3,3	0.33	0	2,2,2	0.04	0
2	EDO	H	601	-	3,3,3	0.16	0	2,2,2	0.20	0
5	ATP	A	508	-	26,33,33	0.92	1 (3%)	31,52,52	1.37	5 (16%)
2	EDO	C	601	-	3,3,3	0.17	0	2,2,2	0.13	0
5	ATP	B	506	-	26,33,33	0.90	1 (3%)	31,52,52	1.38	4 (12%)
2	EDO	E	601	-	3,3,3	0.15	0	2,2,2	0.20	0
2	EDO	L	503	-	3,3,3	0.18	0	2,2,2	0.20	0
2	EDO	G	605	-	3,3,3	0.17	0	2,2,2	0.31	0
2	EDO	C	603	-	3,3,3	0.17	0	2,2,2	0.20	0
6	AKG	D	507	-	9,9,9	1.88	1 (11%)	11,11,11	1.50	2 (18%)
6	AKG	L	504	-	9,9,9	1.73	1 (11%)	11,11,11	1.42	1 (9%)
5	ATP	F	506	-	26,33,33	0.90	1 (3%)	31,52,52	1.36	5 (16%)
6	AKG	H	602	-	9,9,9	2.00	2 (22%)	11,11,11	1.52	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	A	506	-	3,3,3	0.18	0	2,2,2	0.15	0
5	ATP	I	504	-	26,33,33	0.89	1 (3%)	31,52,52	1.27	4 (12%)
3	PEG	J	801	-	6,6,6	0.13	0	5,5,5	0.25	0
9	PG4	D	505	-	12,12,12	0.16	0	11,11,11	0.17	0
3	PEG	G	602	-	5,5,6	0.22	0	4,4,5	0.10	0
2	EDO	B	504	-	3,3,3	0.17	0	2,2,2	0.20	0
5	ATP	K	504	8	26,33,33	0.89	1 (3%)	31,52,52	1.34	5 (16%)
2	EDO	I	502	-	3,3,3	0.15	0	2,2,2	0.19	0
6	AKG	K	503	-	9,9,9	1.98	1 (11%)	11,11,11	1.52	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	J	802	-	-	1/1/1/1	-
5	ATP	J	805	-	-	1/18/38/38	0/3/3/3
5	ATP	L	505	-	-	1/18/38/38	0/3/3/3
5	ATP	E	604	8	-	1/18/38/38	0/3/3/3
2	EDO	B	501	-	-	0/1/1/1	-
3	PEG	A	502	-	-	2/4/4/4	-
6	AKG	B	507	-	-	1/9/9/9	-
2	EDO	A	505	-	-	0/1/1/1	-
3	PEG	A	504	-	-	2/4/4/4	-
2	EDO	A	503	-	-	1/1/1/1	-
5	ATP	D	506	-	-	6/18/38/38	0/3/3/3
2	EDO	F	503	-	-	0/1/1/1	-
2	EDO	I	505	-	-	1/1/1/1	-
6	AKG	F	505	-	-	3/9/9/9	-
2	EDO	J	803	-	-	0/1/1/1	-
6	AKG	E	603	-	-	4/9/9/9	-
6	AKG	G	606	-	-	4/9/9/9	-
2	EDO	F	501	-	-	0/1/1/1	-
7	MOE	B	503	-	-	2/2/2/2	-
2	EDO	I	501	-	-	1/1/1/1	-
3	PEG	G	601	-	-	3/4/4/4	-
2	EDO	L	501	-	-	1/1/1/1	-
3	PEG	G	603	-	-	4/4/4/4	-
5	ATP	G	607	-	-	7/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AKG	A	509	-	-	3/9/9/9	-
3	PEG	D	503	-	-	2/4/4/4	-
2	EDO	D	502	-	-	1/1/1/1	-
5	ATP	C	604	-	-	4/18/38/38	0/3/3/3
6	AKG	J	804	-	-	1/9/9/9	-
2	EDO	F	502	-	-	1/1/1/1	-
2	EDO	F	504	-	-	0/1/1/1	-
3	PEG	D	504	-	-	4/4/4/4	-
3	PEG	G	604	-	-	3/4/4/4	-
6	AKG	I	503	-	-	4/9/9/9	-
5	ATP	H	603	-	-	4/18/38/38	0/3/3/3
2	EDO	B	502	-	-	1/1/1/1	-
9	PG4	D	501	-	-	6/10/10/10	-
4	GOL	A	507	-	-	1/4/4/4	-
2	EDO	L	502	-	-	0/1/1/1	-
6	AKG	C	605	-	-	4/9/9/9	-
3	PEG	K	501	-	-	3/4/4/4	-
2	EDO	C	602	-	-	0/1/1/1	-
7	MOE	F	507	-	-	2/2/2/2	-
2	EDO	A	501	-	-	1/1/1/1	-
2	EDO	H	601	-	-	0/1/1/1	-
5	ATP	A	508	-	-	1/18/38/38	0/3/3/3
2	EDO	C	601	-	-	1/1/1/1	-
5	ATP	B	506	-	-	0/18/38/38	0/3/3/3
2	EDO	E	601	-	-	1/1/1/1	-
2	EDO	L	503	-	-	1/1/1/1	-
2	EDO	G	605	-	-	0/1/1/1	-
2	EDO	C	603	-	-	1/1/1/1	-
6	AKG	D	507	-	-	4/9/9/9	-
6	AKG	L	504	-	-	2/9/9/9	-
5	ATP	F	506	-	-	5/18/38/38	0/3/3/3
6	AKG	H	602	-	-	4/9/9/9	-
2	EDO	A	506	-	-	1/1/1/1	-
5	ATP	I	504	-	-	3/18/38/38	0/3/3/3
3	PEG	J	801	-	-	2/4/4/4	-
9	PG4	D	505	-	-	8/10/10/10	-
3	PEG	G	602	-	-	1/3/3/4	-
2	EDO	B	504	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	K	504	8	-	2/18/38/38	0/3/3/3
2	EDO	I	502	-	-	1/1/1/1	-
6	AKG	K	503	-	-	1/9/9/9	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	603	AKG	C2-C1	-6.78	1.44	1.53
6	C	605	AKG	C2-C1	-6.48	1.44	1.53
6	K	503	AKG	C2-C1	-5.34	1.46	1.53
6	A	509	AKG	C2-C1	-5.25	1.46	1.53
6	F	505	AKG	C2-C1	-5.18	1.46	1.53
6	J	804	AKG	C2-C1	-5.17	1.46	1.53
6	H	602	AKG	C2-C1	-5.04	1.46	1.53
6	G	606	AKG	C2-C1	-4.81	1.47	1.53
6	D	507	AKG	C2-C1	-4.74	1.47	1.53
6	B	507	AKG	C2-C1	-4.39	1.47	1.53
6	I	503	AKG	C2-C1	-4.38	1.47	1.53
6	L	504	AKG	C2-C1	-4.07	1.48	1.53
5	A	508	ATP	C5-C4	2.35	1.47	1.40
5	B	506	ATP	C5-C4	2.35	1.47	1.40
5	D	506	ATP	C5-C4	2.34	1.47	1.40
5	L	505	ATP	C5-C4	2.33	1.47	1.40
5	H	603	ATP	C5-C4	2.32	1.47	1.40
5	I	504	ATP	C5-C4	2.31	1.47	1.40
5	F	506	ATP	C5-C4	2.28	1.47	1.40
5	J	805	ATP	C5-C4	2.27	1.46	1.40
5	C	604	ATP	C5-C4	2.21	1.46	1.40
6	H	602	AKG	O2-C1	-2.20	1.24	1.30
5	G	607	ATP	C5-C4	2.17	1.46	1.40
5	K	504	ATP	C5-C4	2.15	1.46	1.40
6	E	603	AKG	O2-C1	-2.10	1.24	1.30
5	E	604	ATP	C5-C4	2.10	1.46	1.40
6	F	505	AKG	O4-C5	-2.01	1.24	1.30

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	509	AKG	C3-C2-C1	4.11	123.60	115.97
5	E	604	ATP	N3-C2-N1	-3.45	123.29	128.68
5	K	504	ATP	N3-C2-N1	-3.42	123.33	128.68
5	C	604	ATP	PA-O3A-PB	-3.38	121.23	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	805	ATP	N3-C2-N1	-3.34	123.47	128.68
5	H	603	ATP	N3-C2-N1	-3.29	123.53	128.68
5	C	604	ATP	N3-C2-N1	-3.29	123.54	128.68
5	A	508	ATP	PA-O3A-PB	-3.28	121.57	132.83
5	B	506	ATP	PA-O3A-PB	-3.28	121.58	132.83
5	G	607	ATP	N3-C2-N1	-3.25	123.60	128.68
5	L	505	ATP	N3-C2-N1	-3.23	123.63	128.68
5	F	506	ATP	N3-C2-N1	-3.23	123.63	128.68
6	B	507	AKG	O1-C1-C2	-3.17	117.49	121.72
5	I	504	ATP	N3-C2-N1	-3.16	123.74	128.68
6	L	504	AKG	C3-C2-C1	3.15	121.83	115.97
5	H	603	ATP	PB-O3B-PG	-3.15	122.01	132.83
5	B	506	ATP	N3-C2-N1	-3.15	123.75	128.68
5	H	603	ATP	PA-O3A-PB	-3.13	122.10	132.83
5	A	508	ATP	PB-O3B-PG	-3.11	122.15	132.83
5	A	508	ATP	N3-C2-N1	-3.07	123.88	128.68
5	D	506	ATP	N3-C2-N1	-3.05	123.92	128.68
5	G	607	ATP	C4-C5-N7	-3.03	106.24	109.40
5	F	506	ATP	PA-O3A-PB	-3.02	122.47	132.83
6	K	503	AKG	C3-C2-C1	3.00	121.54	115.97
5	D	506	ATP	PB-O3B-PG	-2.98	122.61	132.83
5	L	505	ATP	PA-O3A-PB	-2.95	122.69	132.83
5	C	604	ATP	PB-O3B-PG	-2.95	122.71	132.83
5	A	508	ATP	C4-C5-N7	-2.95	106.33	109.40
5	F	506	ATP	PB-O3B-PG	-2.95	122.72	132.83
6	G	606	AKG	O1-C1-C2	-2.94	117.80	121.72
5	D	506	ATP	PA-O3A-PB	-2.93	122.76	132.83
5	J	805	ATP	C4-C5-N7	-2.91	106.36	109.40
5	E	604	ATP	PB-O3B-PG	-2.89	122.91	132.83
5	B	506	ATP	C4-C5-N7	-2.87	106.40	109.40
5	E	604	ATP	PA-O3A-PB	-2.87	122.99	132.83
5	F	506	ATP	C4-C5-N7	-2.86	106.42	109.40
5	B	506	ATP	PB-O3B-PG	-2.86	123.02	132.83
5	I	504	ATP	PA-O3A-PB	-2.86	123.03	132.83
5	C	604	ATP	C4-C5-N7	-2.84	106.44	109.40
5	D	506	ATP	C4-C5-N7	-2.83	106.45	109.40
5	G	607	ATP	PA-O3A-PB	-2.80	123.23	132.83
5	L	505	ATP	C4-C5-N7	-2.79	106.49	109.40
5	K	504	ATP	PA-O3A-PB	-2.76	123.35	132.83
5	E	604	ATP	C4-C5-N7	-2.74	106.54	109.40
6	G	606	AKG	O2-C1-C2	2.72	121.40	113.97
5	D	506	ATP	O4'-C1'-C2'	-2.70	102.98	106.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	504	ATP	C4-C5-N7	-2.70	106.59	109.40
5	G	607	ATP	PB-O3B-PG	-2.68	123.63	132.83
5	I	504	ATP	PB-O3B-PG	-2.63	123.79	132.83
5	J	805	ATP	PA-O3A-PB	-2.62	123.84	132.83
6	H	602	AKG	O2-C1-C2	2.60	121.10	113.97
5	H	603	ATP	C4-C5-N7	-2.60	106.69	109.40
5	I	504	ATP	C4-C5-N7	-2.59	106.70	109.40
6	D	507	AKG	O2-C1-C2	2.58	121.03	113.97
5	J	805	ATP	PB-O3B-PG	-2.57	124.00	132.83
6	K	503	AKG	O1-C1-C2	-2.55	118.32	121.72
6	H	602	AKG	C3-C2-C1	2.53	120.68	115.97
6	H	602	AKG	O1-C1-C2	-2.52	118.35	121.72
6	B	507	AKG	O2-C1-C2	2.50	120.81	113.97
6	J	804	AKG	C3-C2-C1	2.48	120.57	115.97
5	K	504	ATP	PB-O3B-PG	-2.46	124.39	132.83
5	L	505	ATP	PB-O3B-PG	-2.44	124.47	132.83
5	E	604	ATP	O4'-C1'-C2'	-2.39	103.43	106.93
6	G	606	AKG	C3-C2-C1	2.36	120.35	115.97
5	C	604	ATP	O4'-C1'-C2'	-2.26	103.62	106.93
6	D	507	AKG	O1-C1-C2	-2.24	118.72	121.72
5	J	805	ATP	O4'-C1'-C2'	-2.21	103.70	106.93
5	A	508	ATP	O4'-C1'-C2'	-2.19	103.73	106.93
5	F	506	ATP	O4'-C1'-C2'	-2.15	103.78	106.93
6	A	509	AKG	O2-C1-C2	2.13	119.79	113.97
5	K	504	ATP	C1'-N9-C4	-2.11	122.93	126.64
5	L	505	ATP	O4'-C1'-C2'	-2.05	103.93	106.93
5	L	505	ATP	C2-N1-C6	2.02	122.21	118.75
5	J	805	ATP	C1'-N9-C4	-2.01	123.10	126.64
5	E	604	ATP	C1'-N9-C4	-2.01	123.12	126.64
5	J	805	ATP	C2-N1-C6	2.00	122.18	118.75

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	506	ATP	C5'-O5'-PA-O1A
5	G	607	ATP	PB-O3B-PG-O3G
5	G	607	ATP	C5'-O5'-PA-O3A
5	H	603	ATP	C5'-O5'-PA-O1A
6	A	509	AKG	O2-C1-C2-C3
6	B	507	AKG	O2-C1-C2-C3
6	C	605	AKG	O2-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	D	507	AKG	O2-C1-C2-C3
6	F	505	AKG	O2-C1-C2-C3
6	G	606	AKG	O2-C1-C2-C3
6	H	602	AKG	O2-C1-C2-C3
6	I	503	AKG	O1-C1-C2-C3
6	I	503	AKG	O2-C1-C2-O5
6	I	503	AKG	O2-C1-C2-C3
6	J	804	AKG	O2-C1-C2-C3
6	K	503	AKG	O2-C1-C2-C3
6	L	504	AKG	O2-C1-C2-C3
3	D	503	PEG	C1-C2-O2-C3
9	D	505	PG4	C5-C6-O4-C7
3	A	502	PEG	C1-C2-O2-C3
9	D	505	PG4	O2-C3-C4-O3
5	G	607	ATP	O4'-C4'-C5'-O5'
5	G	607	ATP	C3'-C4'-C5'-O5'
3	G	603	PEG	O2-C3-C4-O4
3	A	504	PEG	O1-C1-C2-O2
3	D	503	PEG	O2-C3-C4-O4
3	K	501	PEG	O1-C1-C2-O2
9	D	505	PG4	O1-C1-C2-O2
3	G	601	PEG	O2-C3-C4-O4
2	F	502	EDO	O1-C1-C2-O2
2	I	501	EDO	O1-C1-C2-O2
2	I	505	EDO	O1-C1-C2-O2
2	L	501	EDO	O1-C1-C2-O2
9	D	501	PG4	C3-C4-O3-C5
3	G	603	PEG	O1-C1-C2-O2
3	A	502	PEG	O1-C1-C2-O2
3	A	504	PEG	O2-C3-C4-O4
3	D	504	PEG	O1-C1-C2-O2
3	J	801	PEG	O1-C1-C2-O2
3	J	801	PEG	O2-C3-C4-O4
7	F	507	MOE	O2'-CA'-CB'-OC'
9	D	501	PG4	O4-C7-C8-O5
9	D	505	PG4	O4-C7-C8-O5
9	D	501	PG4	O3-C5-C6-O4
2	A	501	EDO	O1-C1-C2-O2
2	B	502	EDO	O1-C1-C2-O2
2	C	603	EDO	O1-C1-C2-O2
2	I	502	EDO	O1-C1-C2-O2
5	F	506	ATP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	504	PEG	O2-C3-C4-O4
5	C	604	ATP	O4'-C4'-C5'-O5'
2	B	504	EDO	O1-C1-C2-O2
2	D	502	EDO	O1-C1-C2-O2
3	D	504	PEG	C4-C3-O2-C2
3	G	601	PEG	C4-C3-O2-C2
3	G	604	PEG	C4-C3-O2-C2
3	K	501	PEG	C4-C3-O2-C2
5	A	508	ATP	PB-O3B-PG-O3G
5	H	603	ATP	PB-O3B-PG-O3G
9	D	505	PG4	C1-C2-O2-C3
3	G	604	PEG	C1-C2-O2-C3
4	A	507	GOL	O2-C2-C3-O3
5	D	506	ATP	C5'-O5'-PA-O3A
5	F	506	ATP	C5'-O5'-PA-O3A
3	G	604	PEG	O2-C3-C4-O4
9	D	505	PG4	C6-C5-O3-C4
5	I	504	ATP	PB-O3A-PA-O1A
7	B	503	MOE	CA'-CB'-OC'-CD'
5	D	506	ATP	C5'-O5'-PA-O2A
5	G	607	ATP	C5'-O5'-PA-O1A
5	G	607	ATP	C5'-O5'-PA-O2A
6	A	509	AKG	O1-C1-C2-O5
6	C	605	AKG	O1-C1-C2-O5
6	D	507	AKG	O1-C1-C2-O5
6	G	606	AKG	O1-C1-C2-O5
6	H	602	AKG	O1-C1-C2-O5
6	I	503	AKG	O1-C1-C2-O5
5	C	604	ATP	C3'-C4'-C5'-O5'
6	A	509	AKG	O1-C1-C2-C3
6	C	605	AKG	O1-C1-C2-C3
6	D	507	AKG	O1-C1-C2-C3
6	E	603	AKG	O1-C1-C2-C3
6	G	606	AKG	O1-C1-C2-C3
6	H	602	AKG	O1-C1-C2-C3
6	L	504	AKG	O1-C1-C2-C3
7	F	507	MOE	CA'-CB'-OC'-CD'
3	G	601	PEG	C1-C2-O2-C3
3	D	504	PEG	C1-C2-O2-C3
3	G	602	PEG	O2-C3-C4-O4
2	A	503	EDO	O1-C1-C2-O2
9	D	501	PG4	C4-C3-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	605	AKG	O2-C1-C2-O5
6	D	507	AKG	O2-C1-C2-O5
6	E	603	AKG	O2-C1-C2-O5
6	G	606	AKG	O2-C1-C2-O5
6	H	602	AKG	O2-C1-C2-O5
5	D	506	ATP	PB-O3A-PA-O1A
5	F	506	ATP	PG-O3B-PB-O2B
5	K	504	ATP	PG-O3B-PB-O2B
9	D	505	PG4	C3-C4-O3-C5
5	D	506	ATP	PB-O3B-PG-O1G
7	B	503	MOE	O2'-CA'-CB'-OC'
5	G	607	ATP	PB-O3A-PA-O1A
2	C	601	EDO	O1-C1-C2-O2
2	L	503	EDO	O1-C1-C2-O2
3	G	603	PEG	C1-C2-O2-C3
6	F	505	AKG	C3-C4-C5-O3
6	E	603	AKG	O2-C1-C2-C3
9	D	505	PG4	O3-C5-C6-O4
5	H	603	ATP	O4'-C4'-C5'-O5'
5	H	603	ATP	C3'-C4'-C5'-O5'
2	A	506	EDO	O1-C1-C2-O2
2	E	601	EDO	O1-C1-C2-O2
2	J	802	EDO	O1-C1-C2-O2
5	D	506	ATP	PB-O3B-PG-O2G
5	D	506	ATP	PB-O3B-PG-O3G
3	G	603	PEG	C4-C3-O2-C2
6	F	505	AKG	C3-C4-C5-O4
5	C	604	ATP	PG-O3B-PB-O2B
5	E	604	ATP	PG-O3B-PB-O2B
5	F	506	ATP	PG-O3B-PB-O1B
5	I	504	ATP	PG-O3B-PB-O2B
5	I	504	ATP	PB-O3A-PA-O2A
5	J	805	ATP	PG-O3B-PB-O2B
5	L	505	ATP	PG-O3B-PB-O2B
3	K	501	PEG	O2-C3-C4-O4
5	C	604	ATP	C5'-O5'-PA-O1A
5	K	504	ATP	C5'-O5'-PA-O1A
6	E	603	AKG	O1-C1-C2-O5
9	D	501	PG4	C1-C2-O2-C3
9	D	501	PG4	O2-C3-C4-O3

There are no ring outliers.

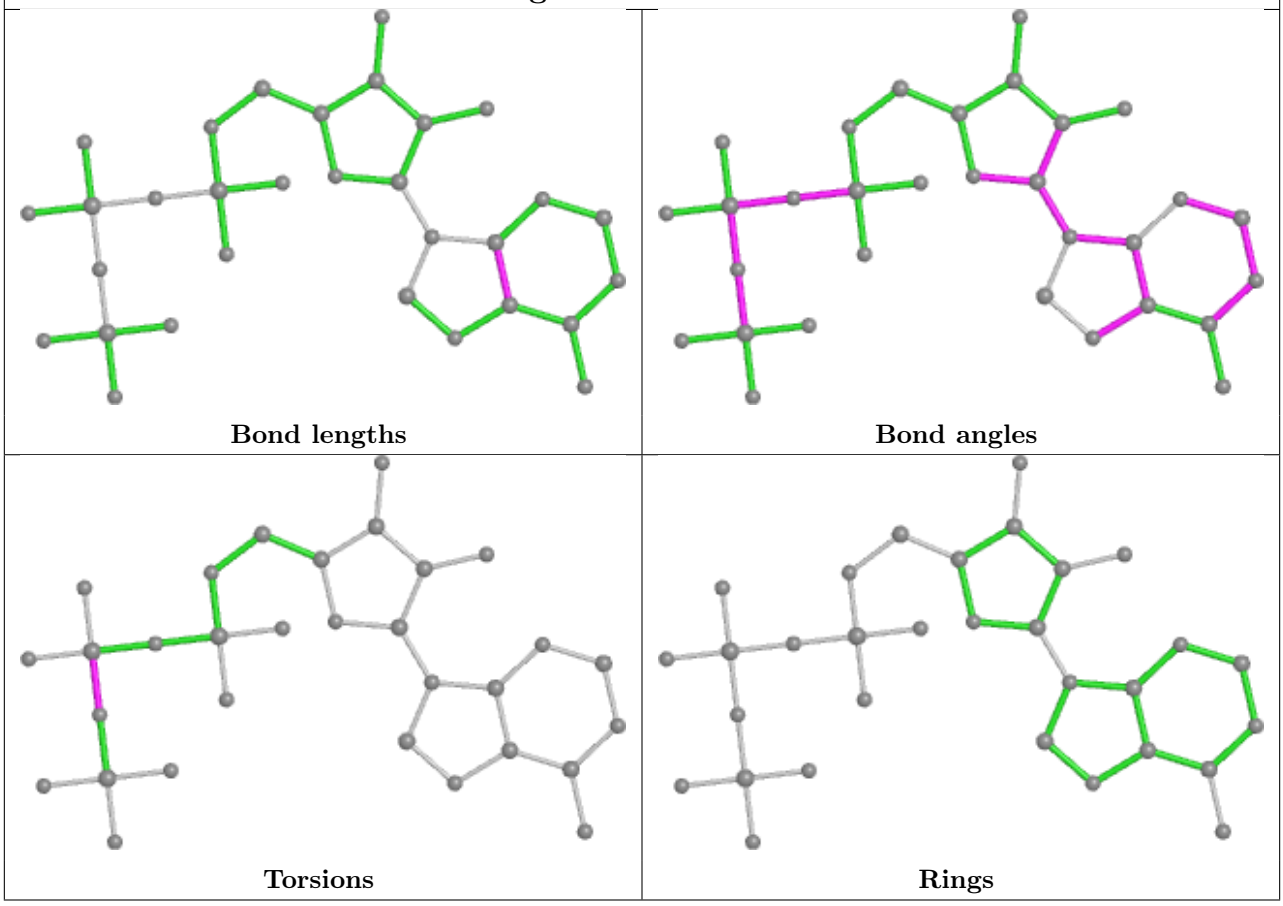
31 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	805	ATP	2	0
5	L	505	ATP	2	0
5	E	604	ATP	1	0
3	A	504	PEG	1	0
5	D	506	ATP	2	0
2	F	503	EDO	2	0
2	J	803	EDO	1	0
7	B	503	MOE	1	0
2	I	501	EDO	1	0
3	G	601	PEG	2	0
3	G	603	PEG	2	0
3	D	503	PEG	1	0
2	D	502	EDO	1	0
5	C	604	ATP	2	0
3	D	504	PEG	3	0
3	G	604	PEG	1	0
5	H	603	ATP	2	0
9	D	501	PG4	6	0
4	A	507	GOL	1	0
3	K	501	PEG	4	0
2	A	501	EDO	2	0
2	H	601	EDO	1	0
5	A	508	ATP	1	0
5	B	506	ATP	2	0
2	C	603	EDO	2	0
5	F	506	ATP	1	0
5	I	504	ATP	3	0
3	J	801	PEG	1	0
9	D	505	PG4	2	0
3	G	602	PEG	1	0
5	K	504	ATP	2	0

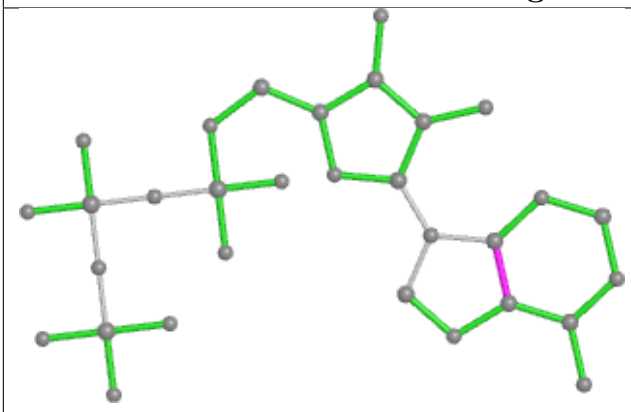
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

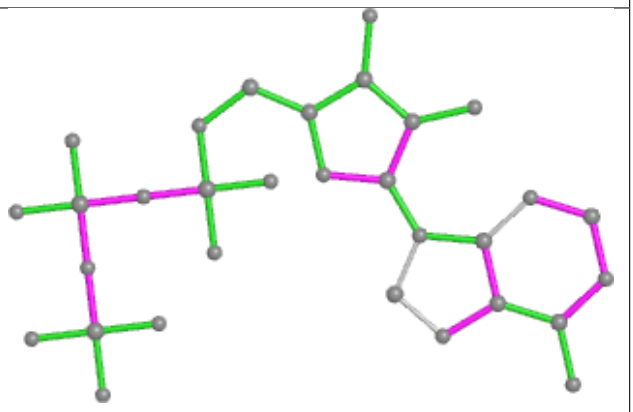
Ligand ATP J 805



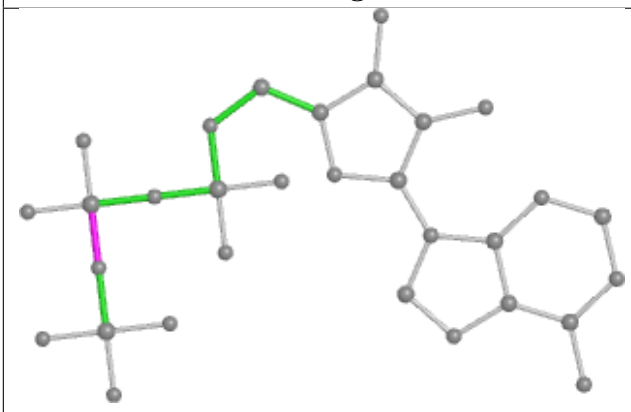
Ligand ATP L 505



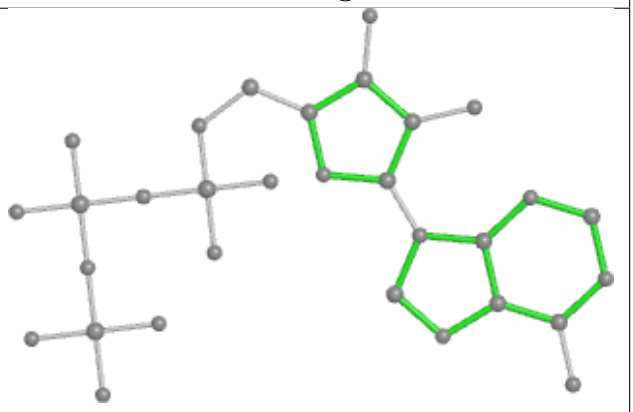
Bond lengths



Bond angles

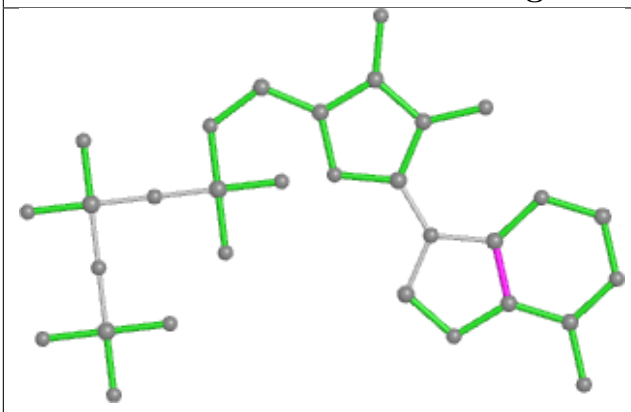


Torsions

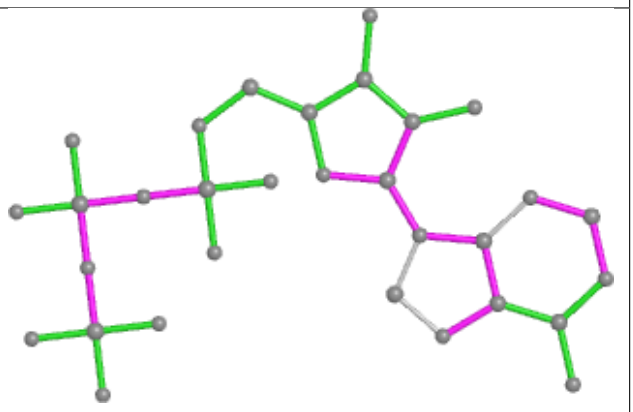


Rings

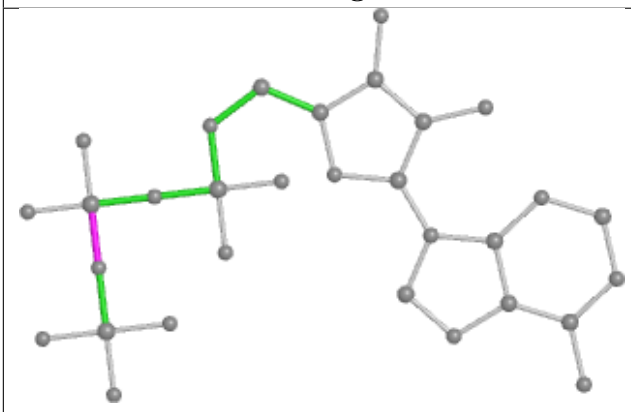
Ligand ATP E 604



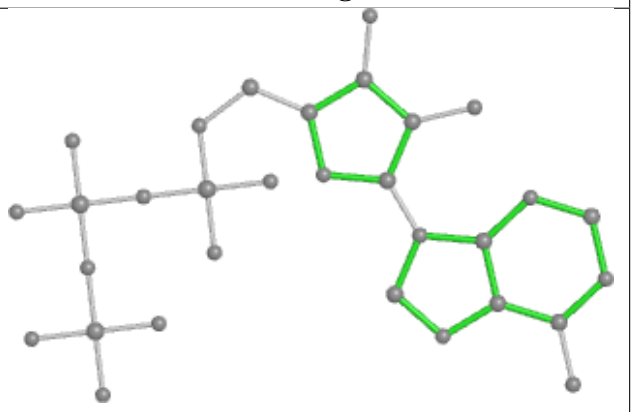
Bond lengths



Bond angles

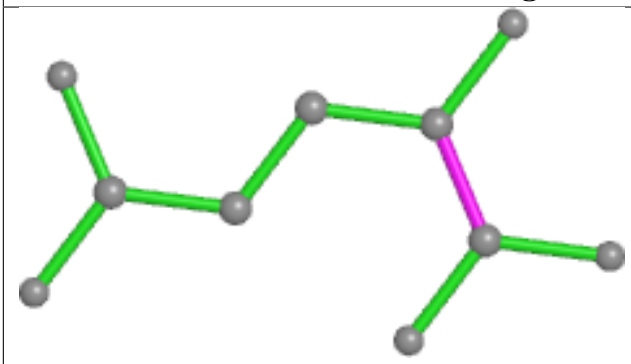


Torsions

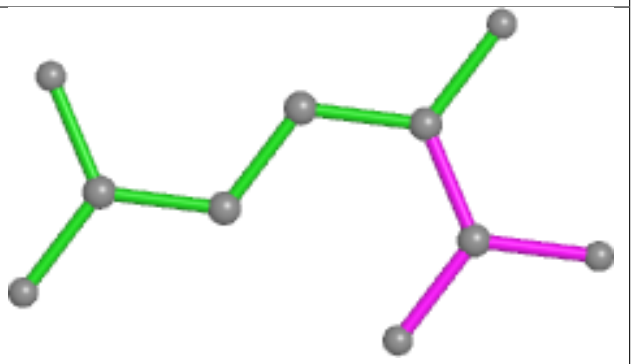


Rings

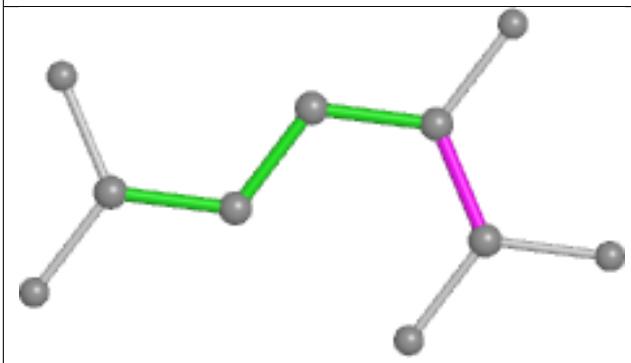
Ligand AKG B 507



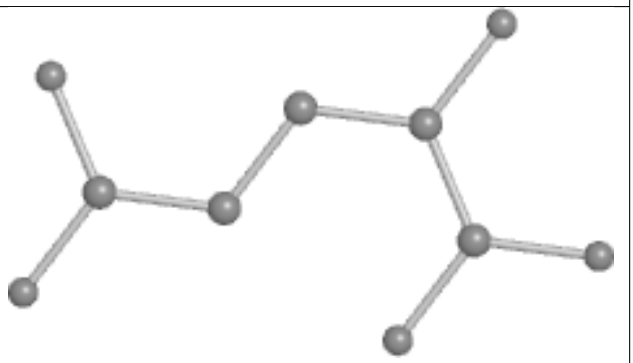
Bond lengths



Bond angles

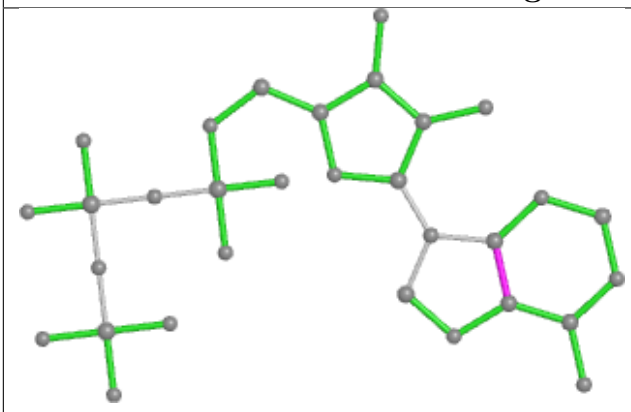


Torsions

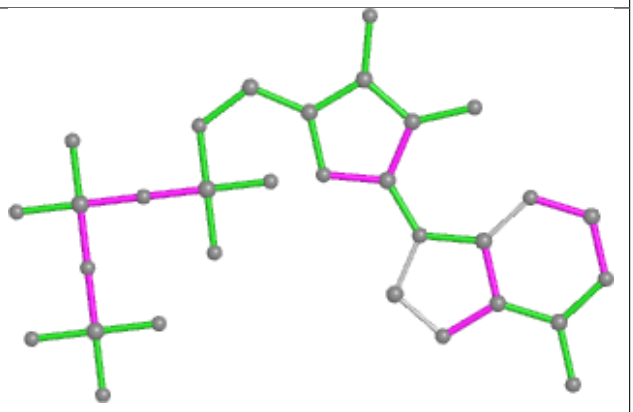


Rings

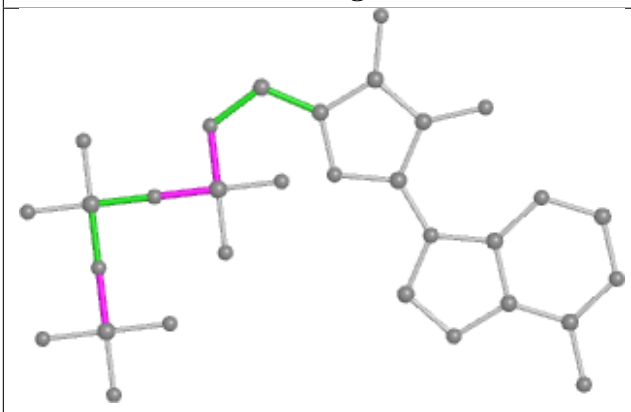
Ligand ATP D 506



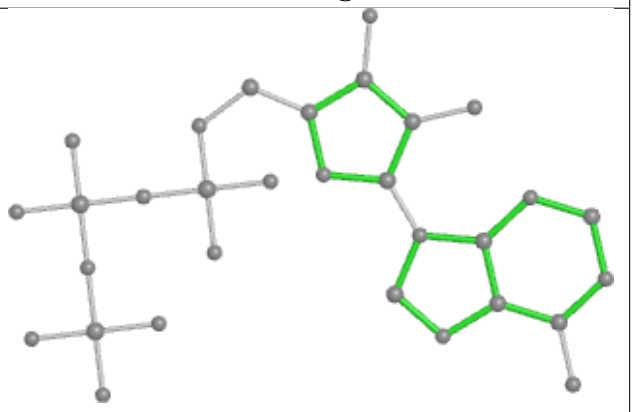
Bond lengths



Bond angles

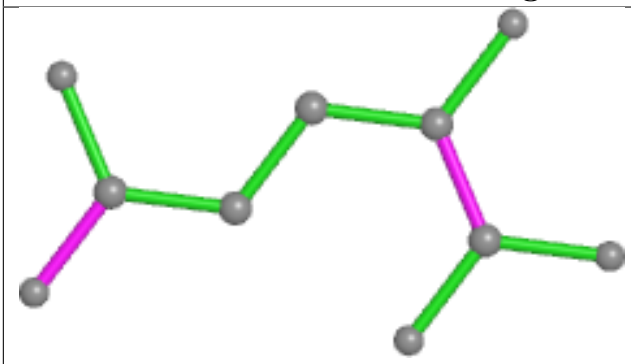


Torsions

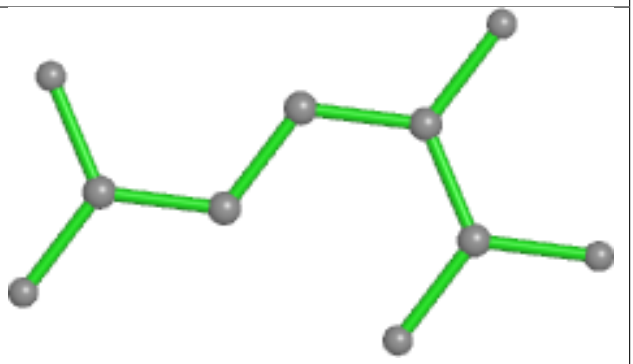


Rings

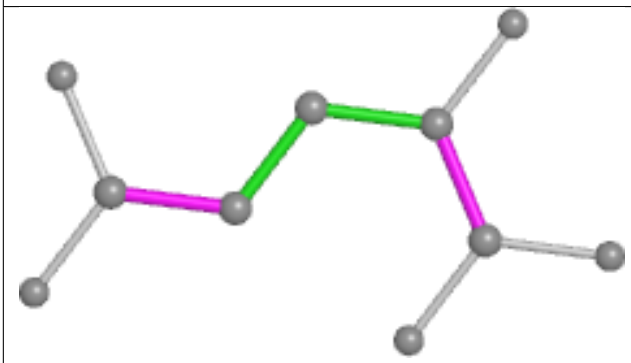
Ligand AKG F 505



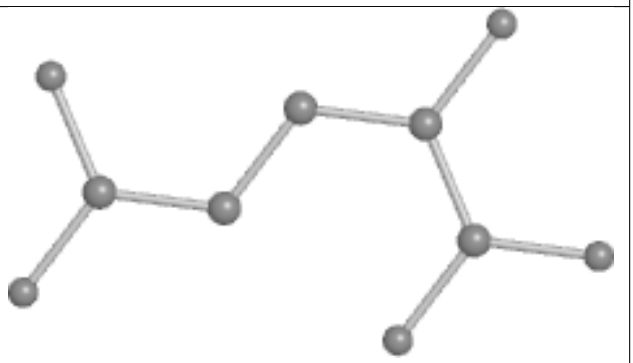
Bond lengths



Bond angles

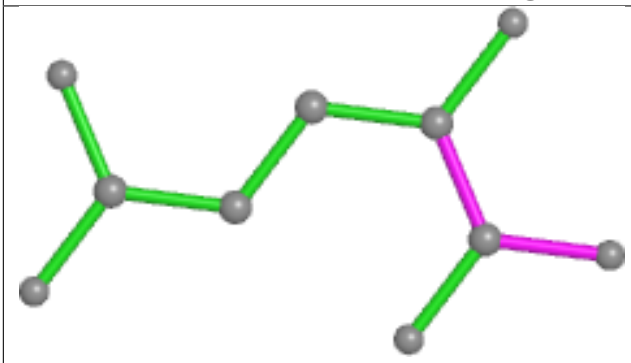


Torsions

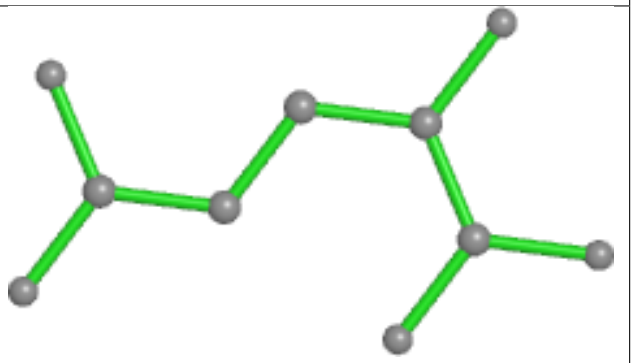


Rings

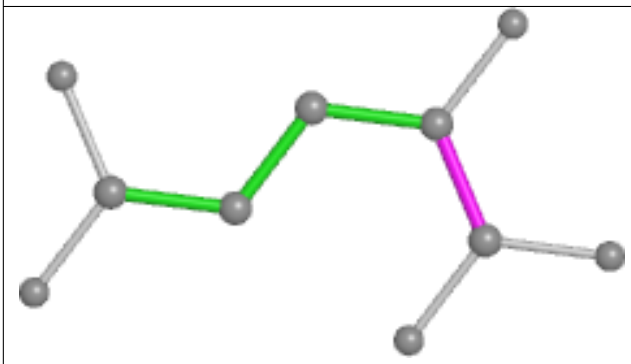
Ligand AKG E 603



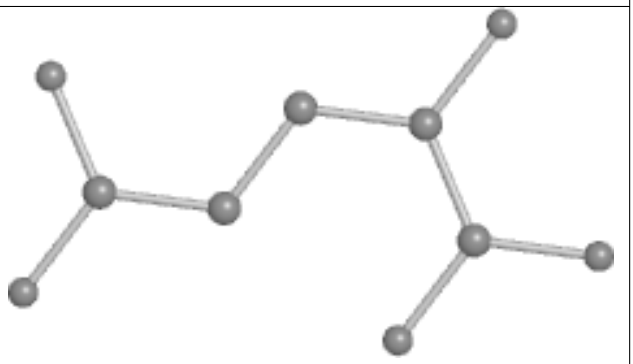
Bond lengths



Bond angles

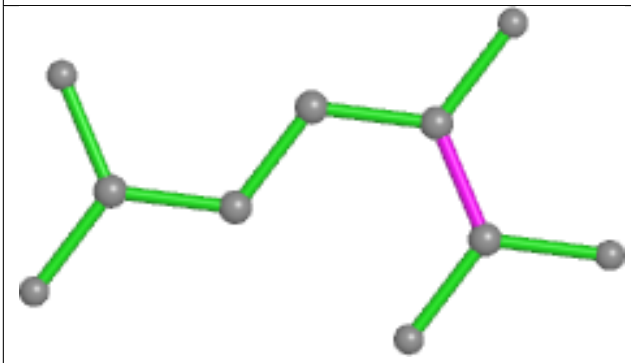


Torsions

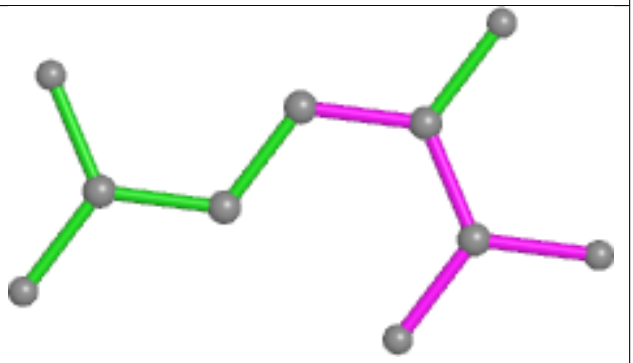


Rings

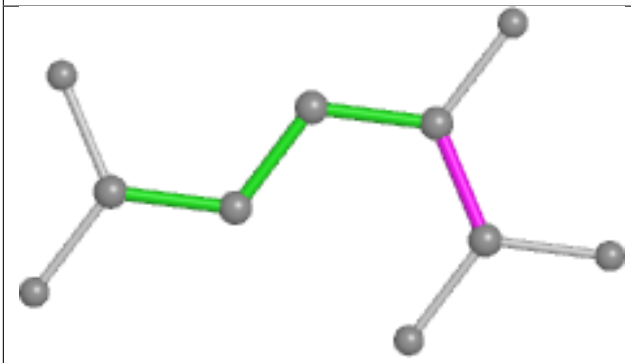
Ligand AKG G 606



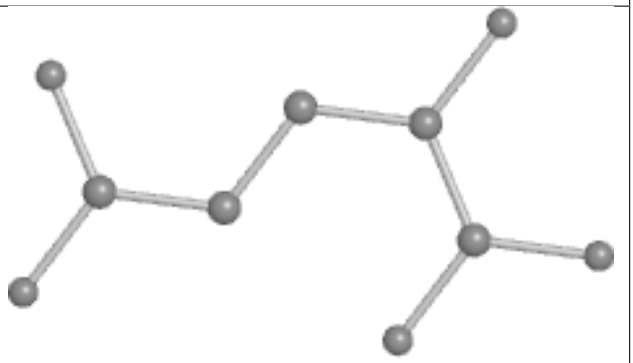
Bond lengths



Bond angles

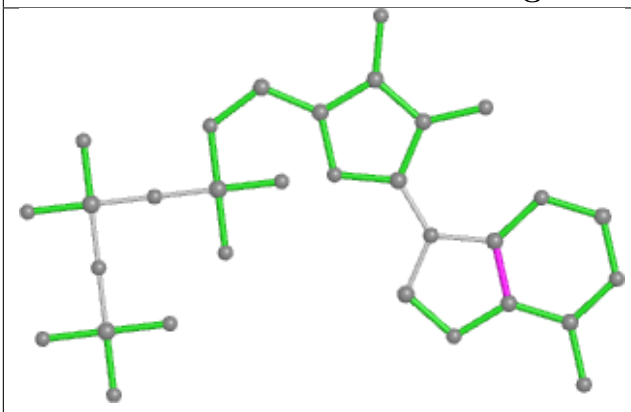


Torsions

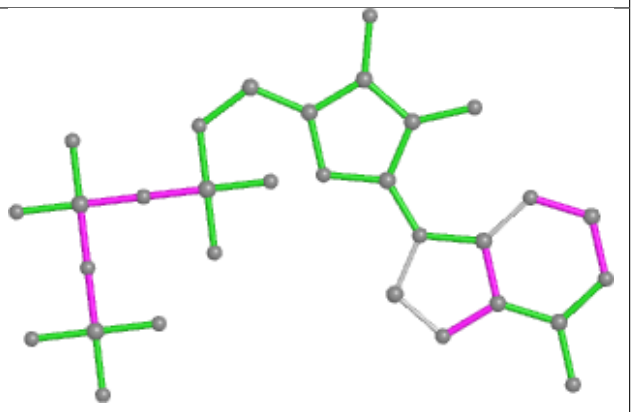


Rings

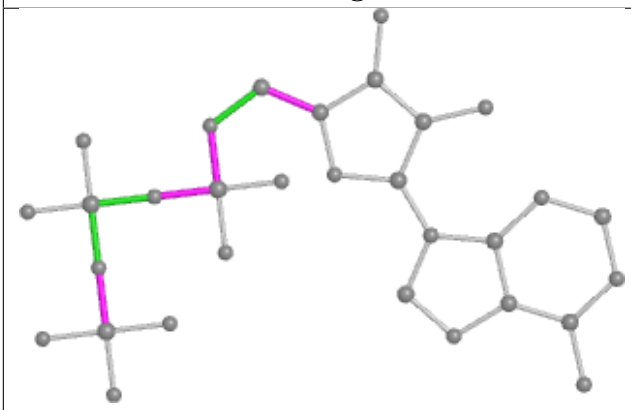
Ligand ATP G 607



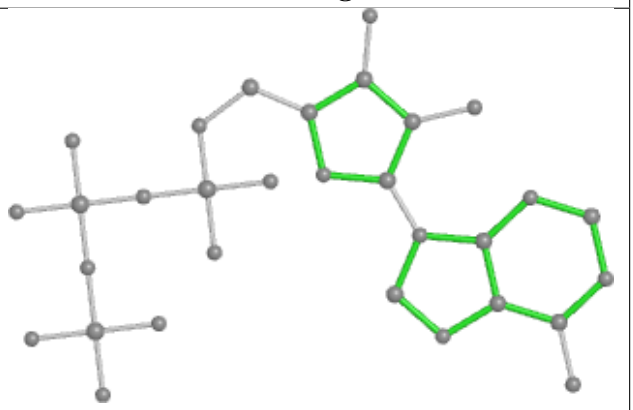
Bond lengths



Bond angles

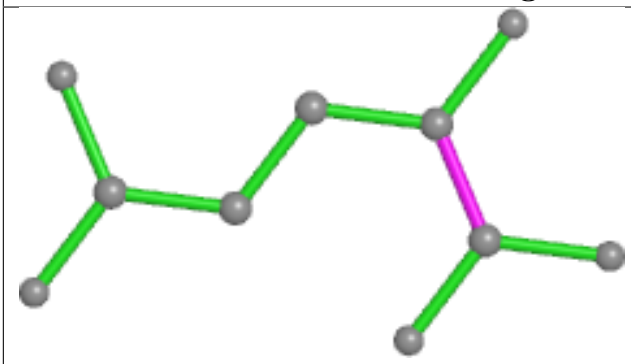


Torsions

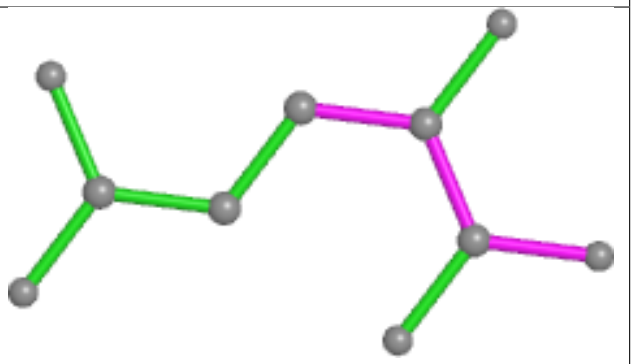


Rings

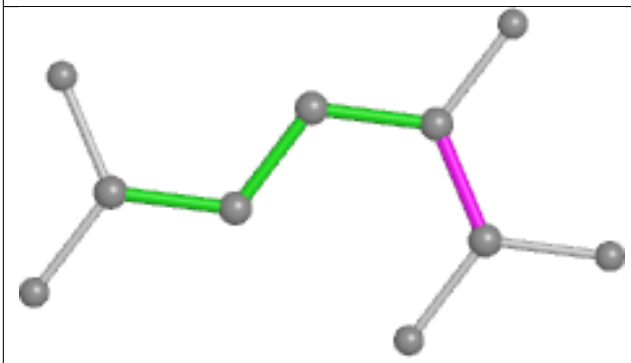
Ligand AKG A 509



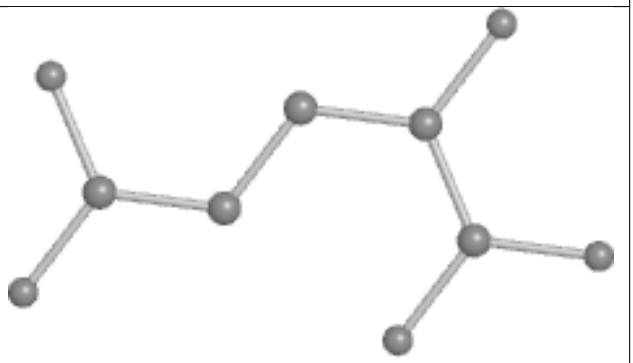
Bond lengths



Bond angles

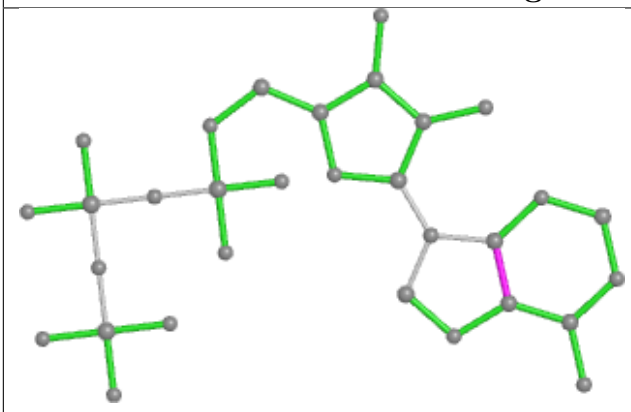


Torsions

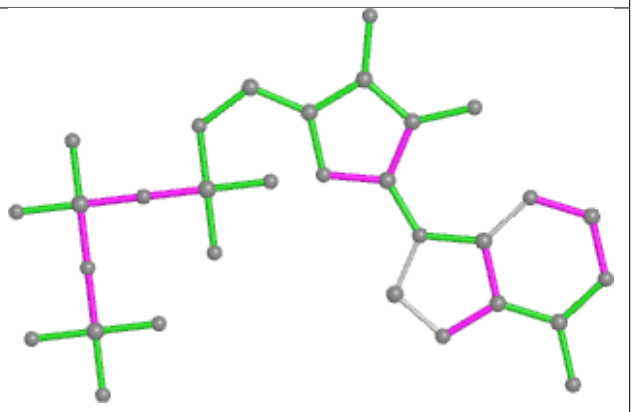


Rings

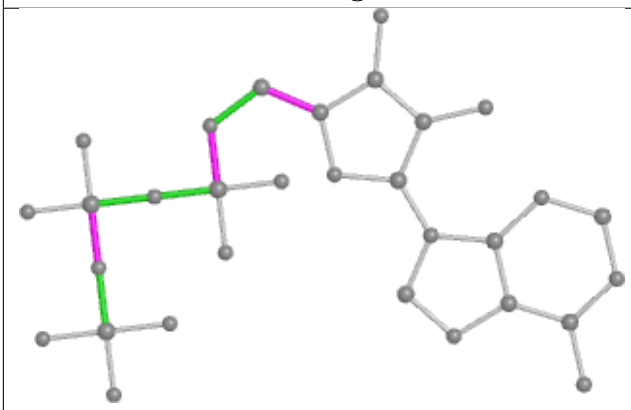
Ligand ATP C 604



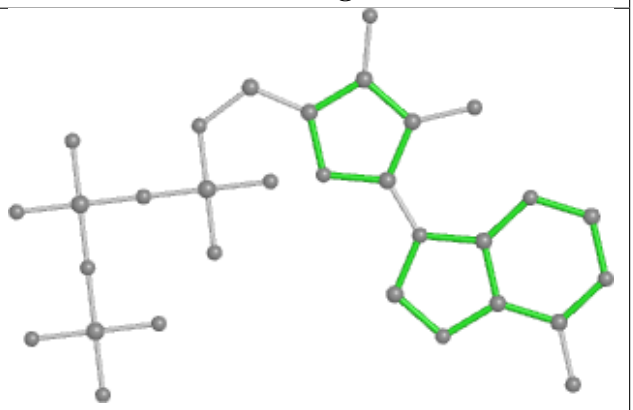
Bond lengths



Bond angles

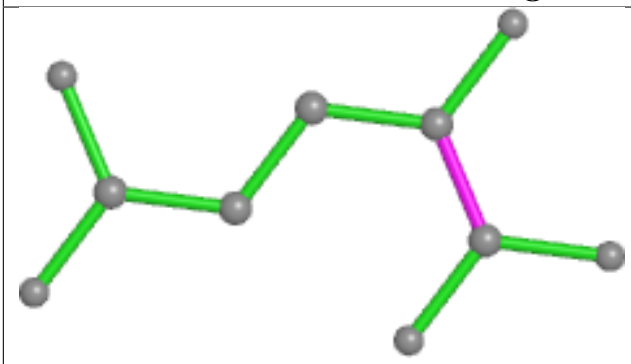


Torsions

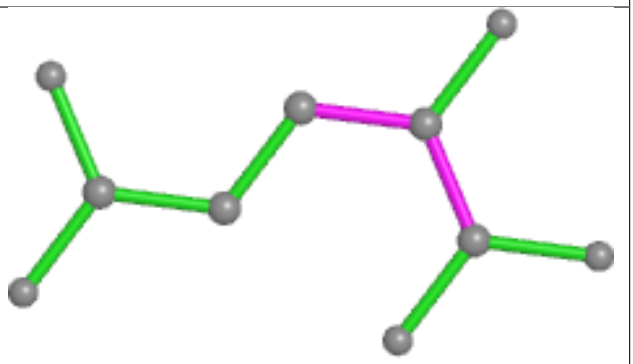


Rings

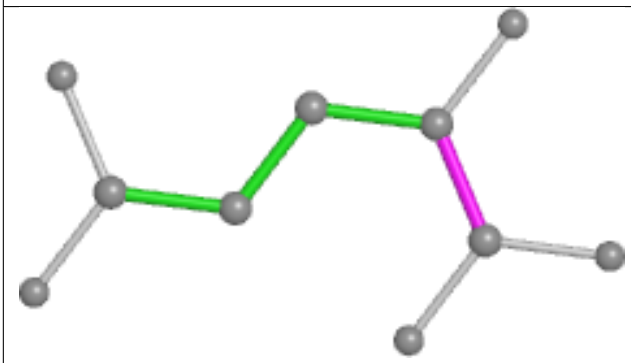
Ligand AKG J 804



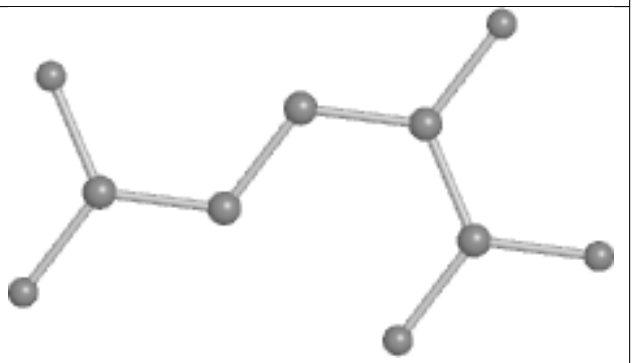
Bond lengths



Bond angles

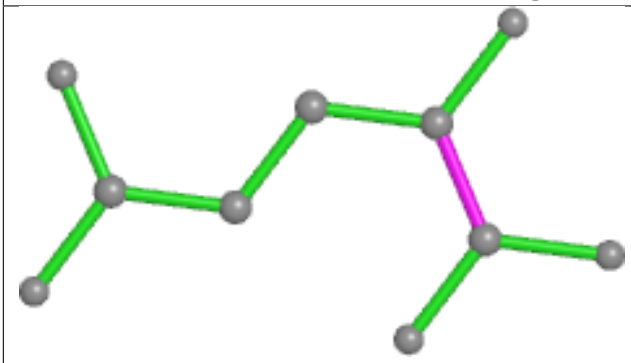


Torsions

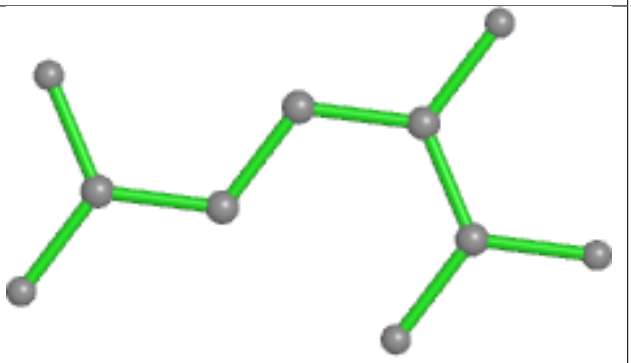


Rings

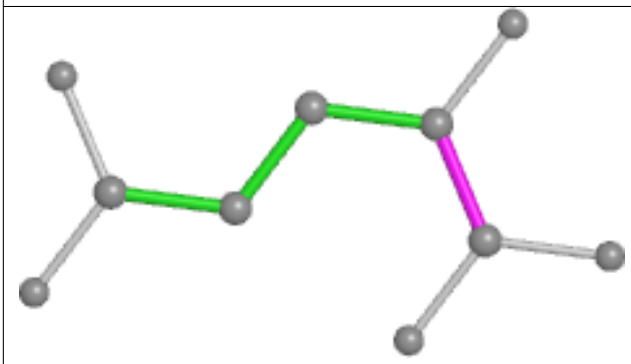
Ligand AKG I 503



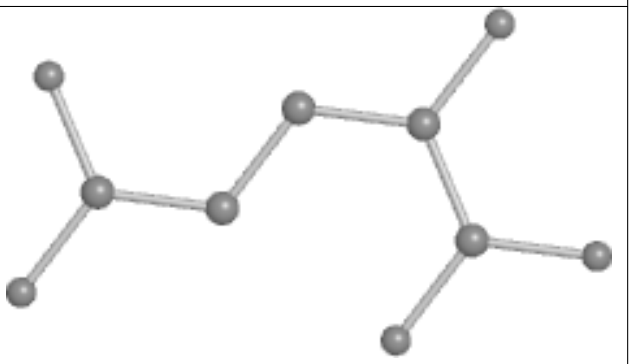
Bond lengths



Bond angles

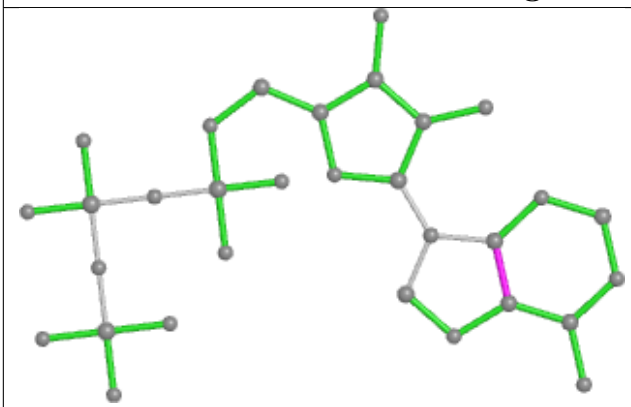


Torsions

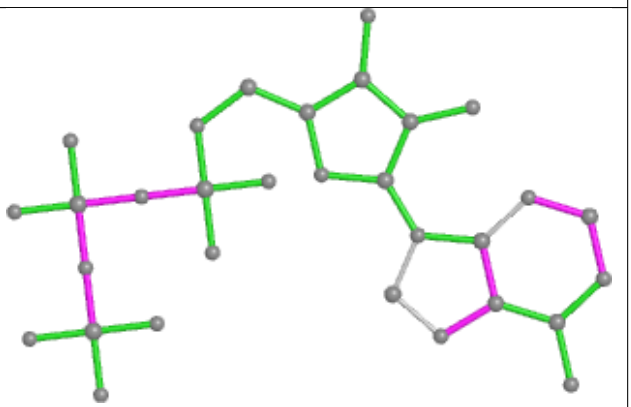


Rings

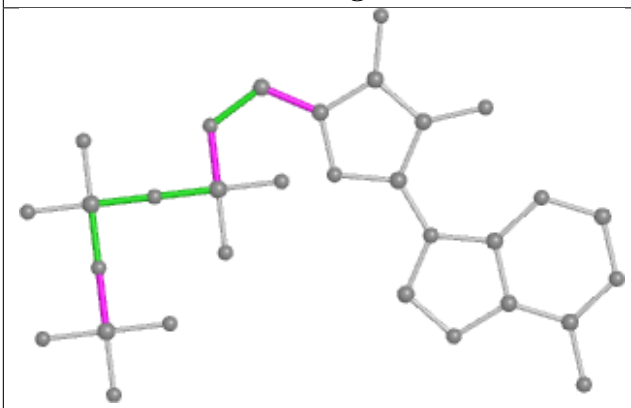
Ligand ATP H 603



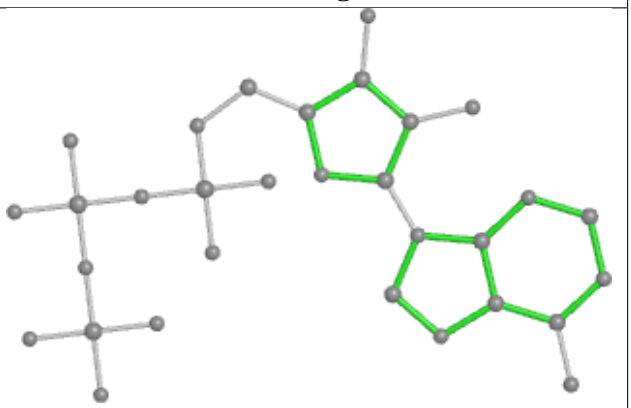
Bond lengths



Bond angles

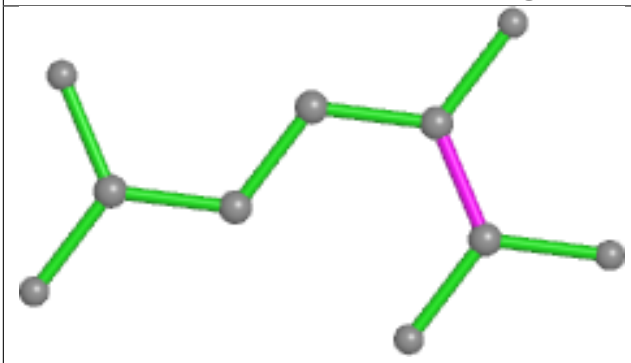


Torsions

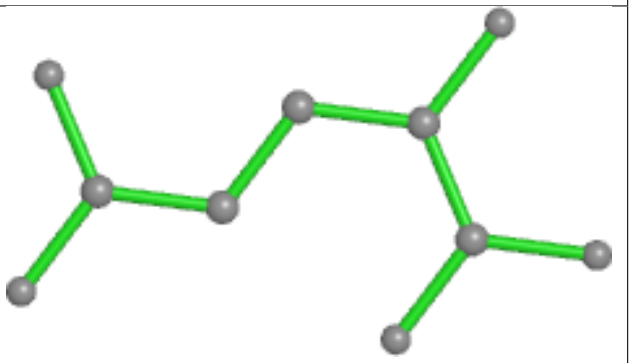


Rings

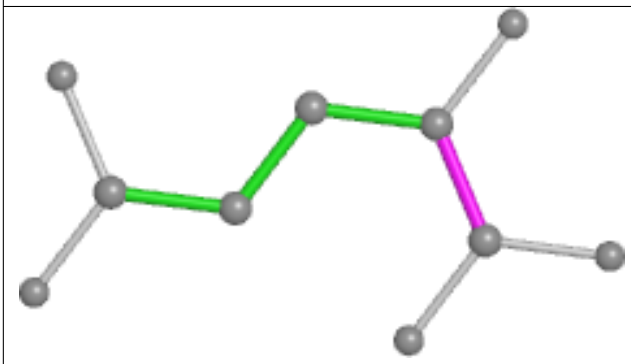
Ligand AKG C 605



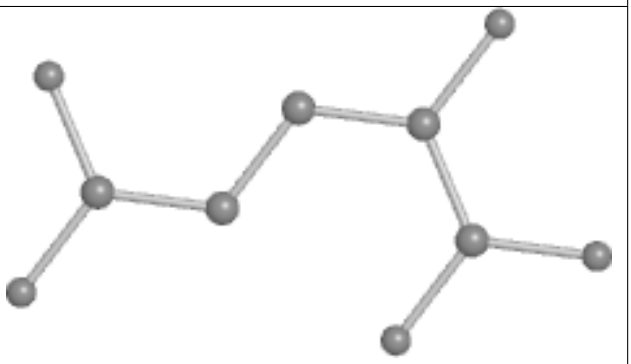
Bond lengths



Bond angles

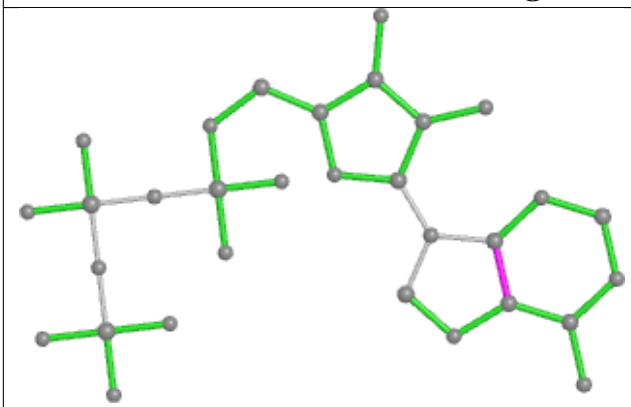


Torsions

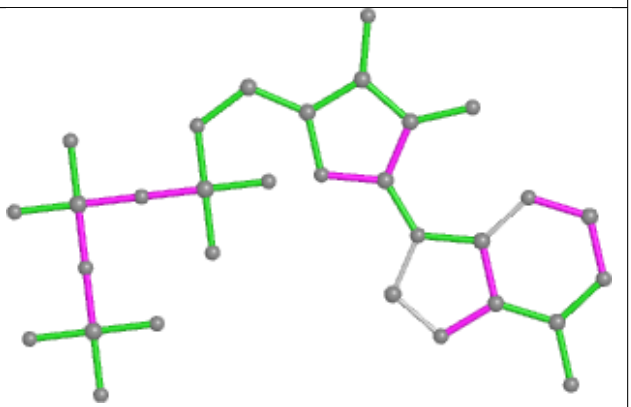


Rings

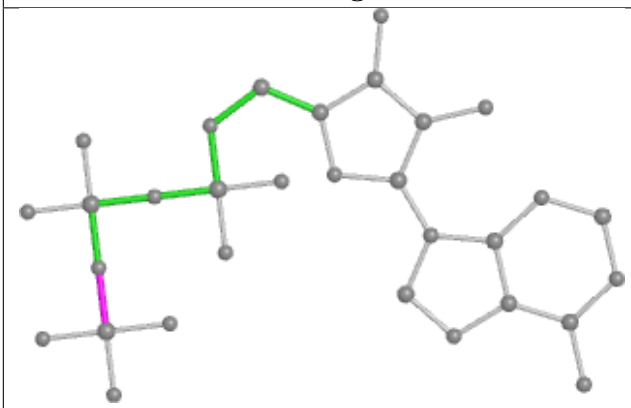
Ligand ATP A 508



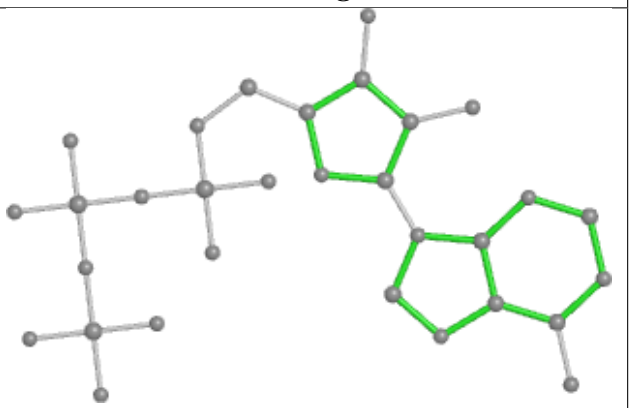
Bond lengths



Bond angles

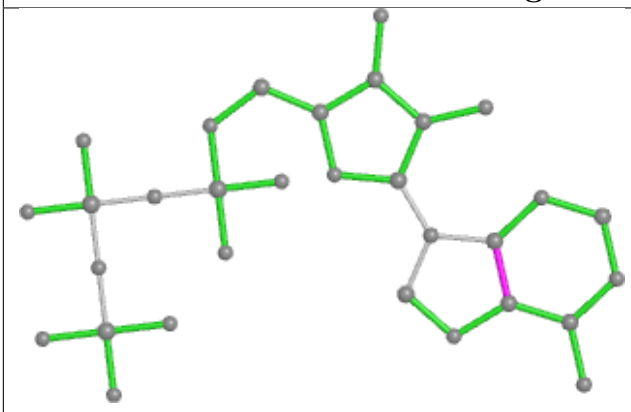


Torsions

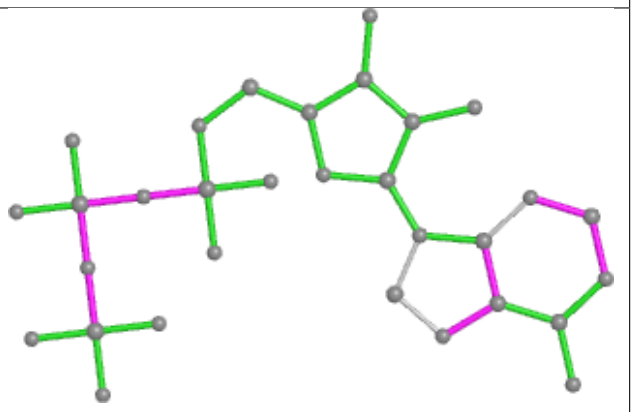


Rings

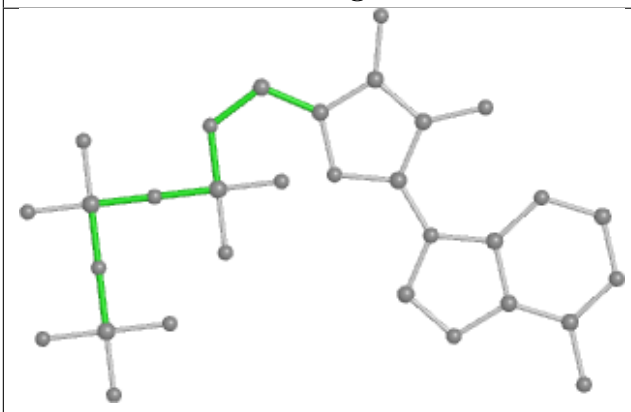
Ligand ATP B 506



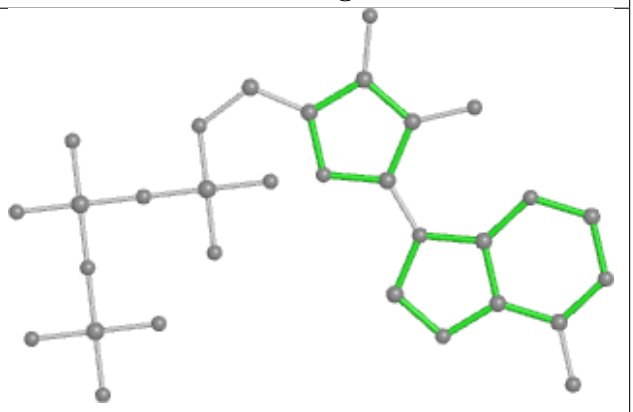
Bond lengths



Bond angles

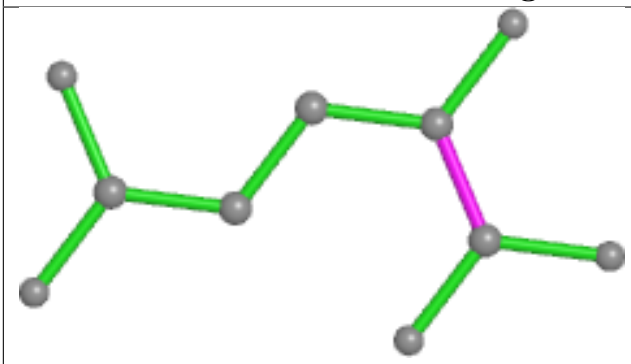


Torsions

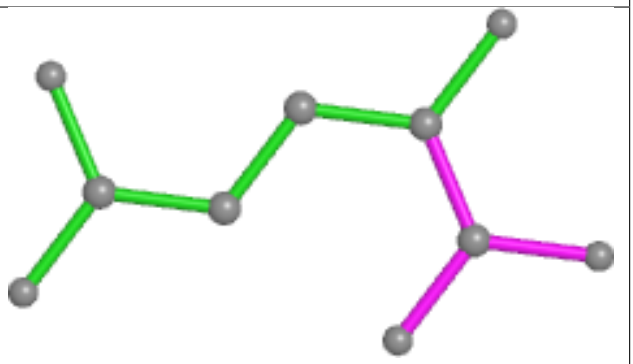


Rings

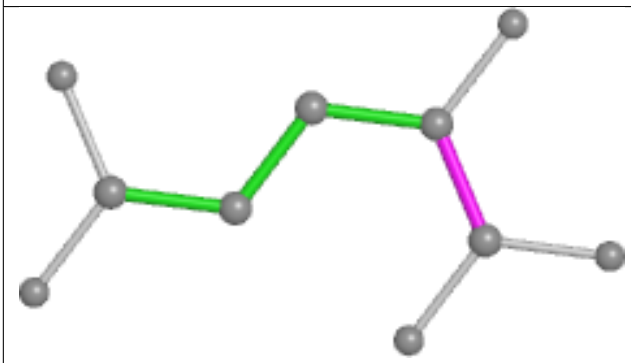
Ligand AKG D 507



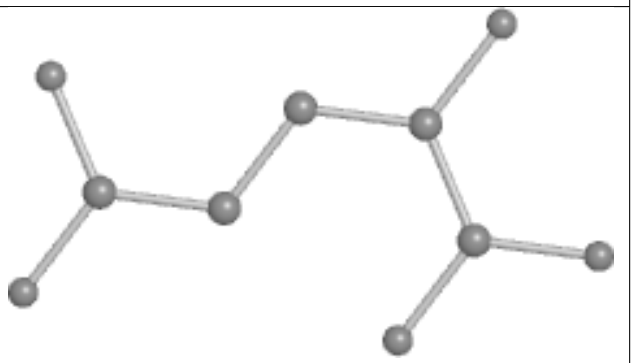
Bond lengths



Bond angles

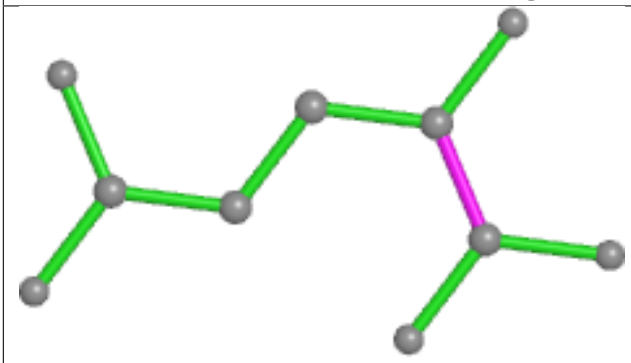


Torsions

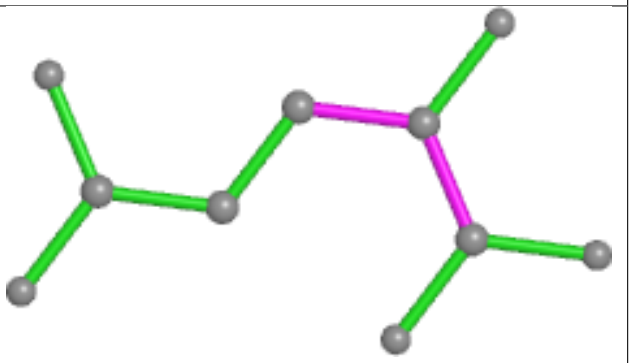


Rings

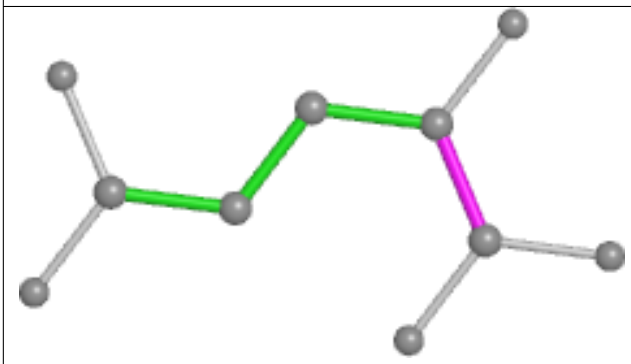
Ligand AKG L 504



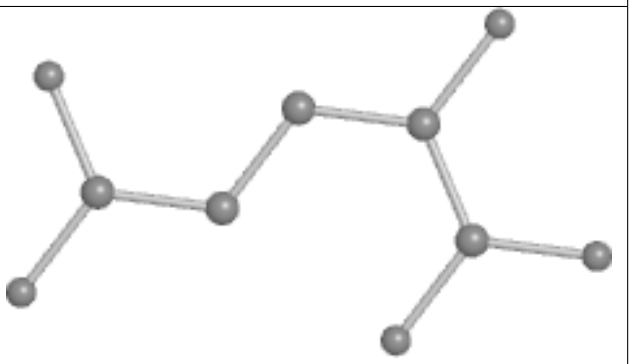
Bond lengths



Bond angles

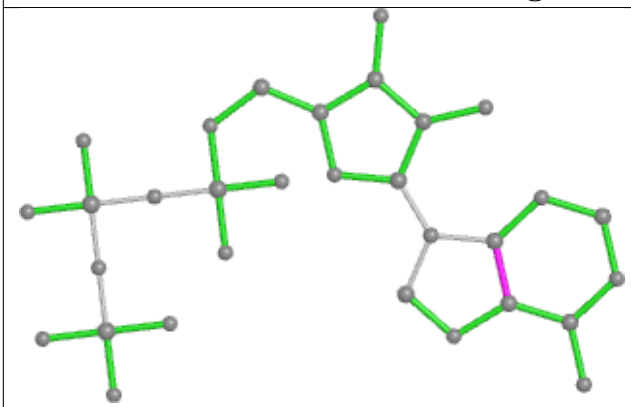


Torsions

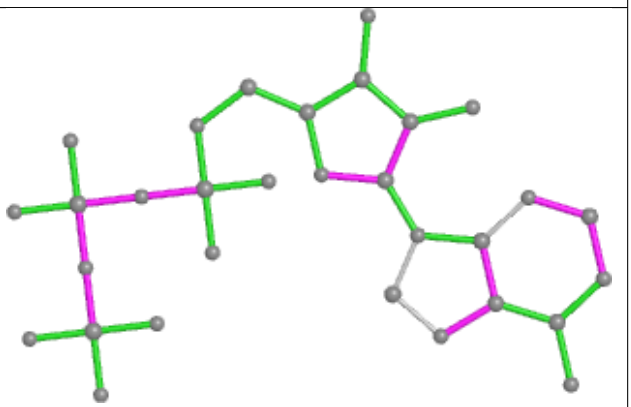


Rings

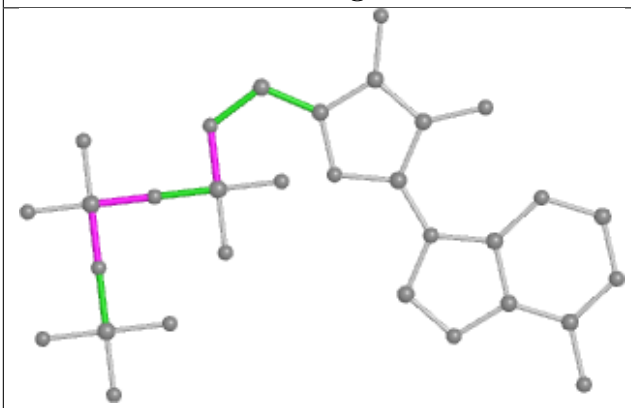
Ligand ATP F 506



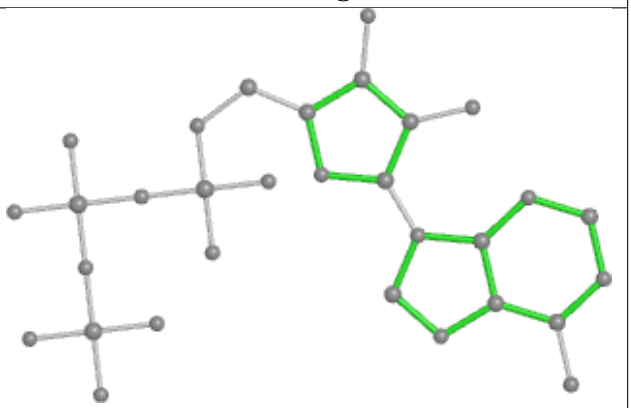
Bond lengths



Bond angles

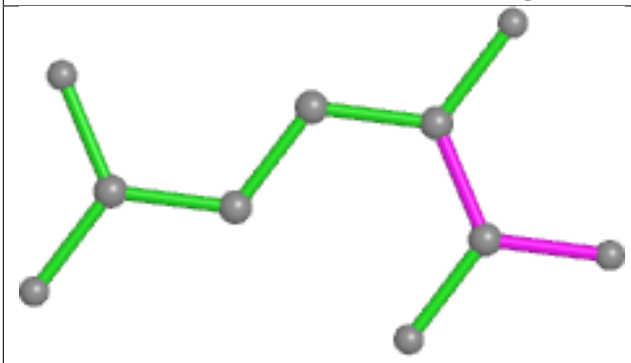


Torsions

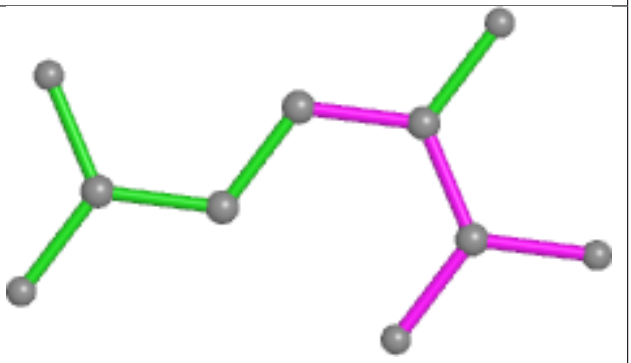


Rings

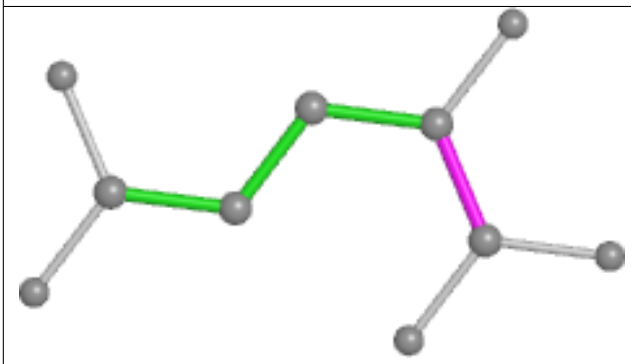
Ligand AKG H 602



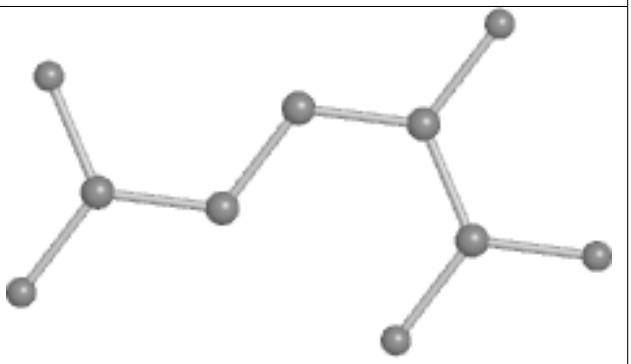
Bond lengths



Bond angles

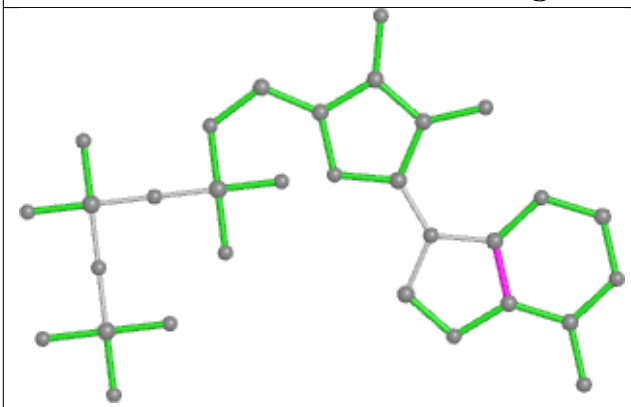


Torsions

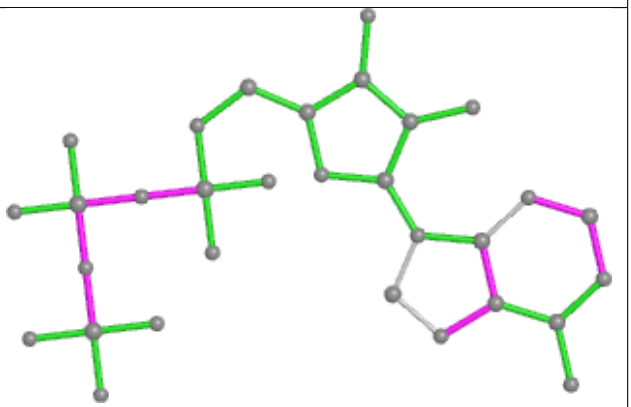


Rings

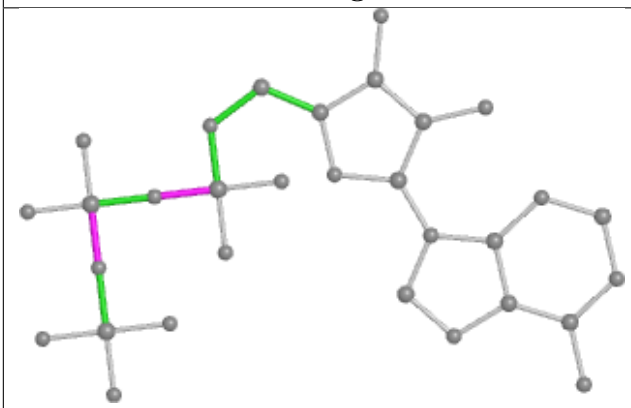
Ligand ATP I 504



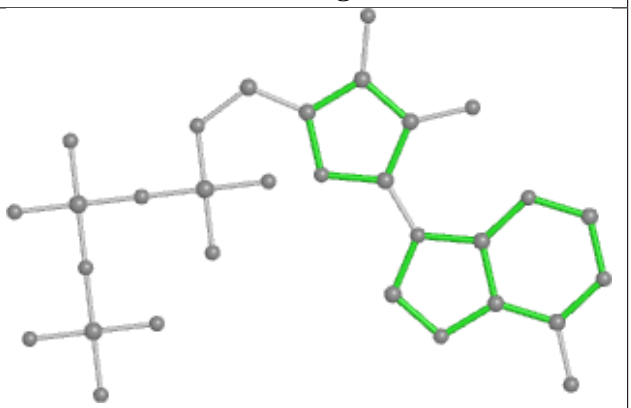
Bond lengths



Bond angles

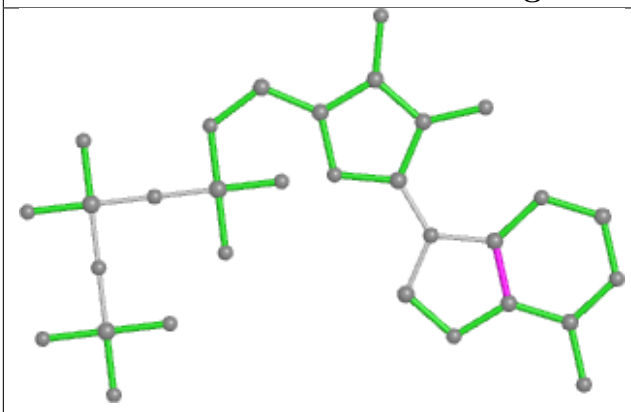


Torsions

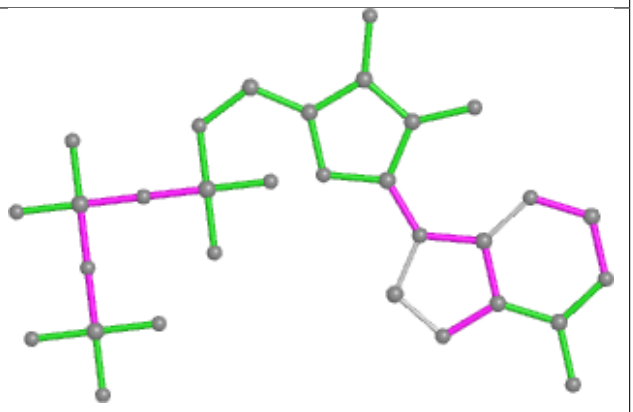


Rings

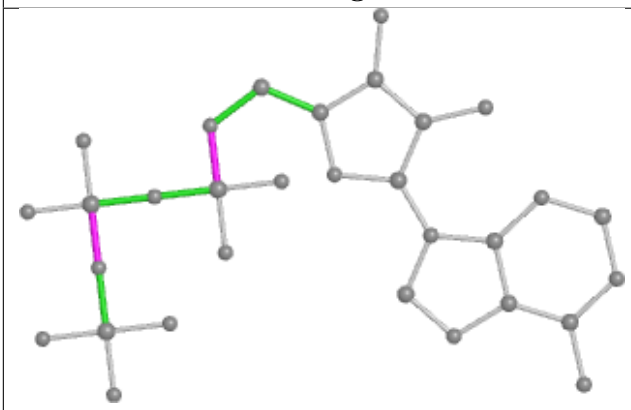
Ligand ATP K 504



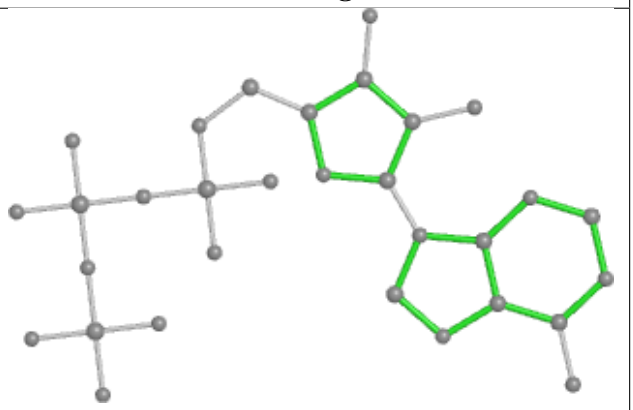
Bond lengths



Bond angles

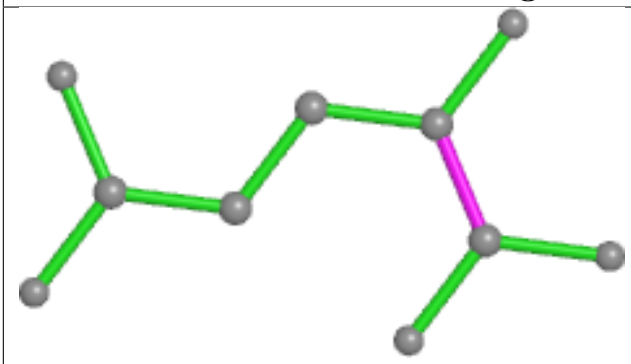


Torsions

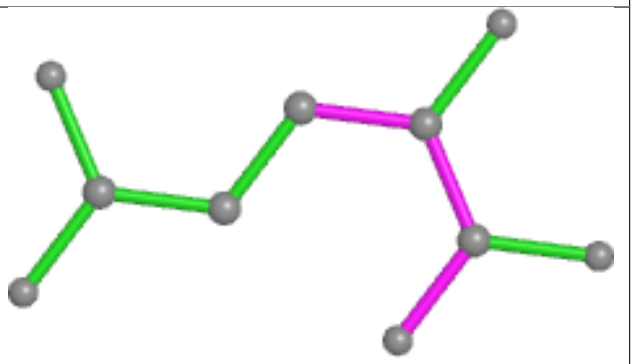


Rings

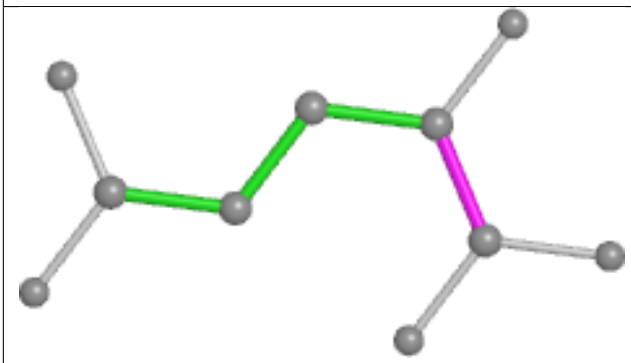
Ligand AKG K 503



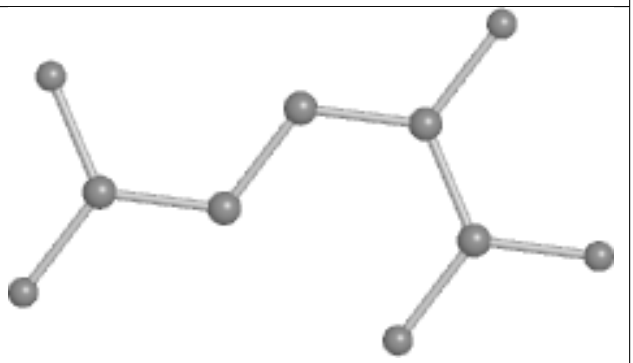
Bond lengths



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	447/448 (99%)	-0.31	2 (0%) 92 94	22, 33, 58, 81	0
1	B	447/448 (99%)	-0.36	1 (0%) 95 96	21, 34, 58, 78	0
1	C	447/448 (99%)	-0.34	2 (0%) 92 94	22, 35, 62, 78	0
1	D	447/448 (99%)	-0.31	2 (0%) 92 94	20, 32, 58, 76	1 (0%)
1	E	447/448 (99%)	-0.33	3 (0%) 87 90	21, 33, 59, 78	0
1	F	447/448 (99%)	-0.33	2 (0%) 92 94	22, 34, 57, 79	1 (0%)
1	G	447/448 (99%)	-0.32	6 (1%) 77 81	22, 36, 63, 83	0
1	H	447/448 (99%)	-0.24	5 (1%) 80 84	23, 35, 68, 89	0
1	I	447/448 (99%)	-0.31	3 (0%) 87 90	24, 36, 62, 81	0
1	J	447/448 (99%)	-0.34	1 (0%) 95 96	21, 32, 58, 79	0
1	K	447/448 (99%)	-0.30	0 100 100	23, 34, 58, 75	0
1	L	447/448 (99%)	-0.31	2 (0%) 92 94	23, 35, 60, 80	0
All	All	5364/5376 (99%)	-0.32	29 (0%) 91 93	20, 34, 61, 89	2 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	2	SER	4.2
1	L	2	SER	4.2
1	F	2	SER	4.1
1	C	2	SER	4.0
1	D	2	SER	3.2
1	G	388	LEU	2.9
1	H	388	LEU	2.7
1	G	387	GLU	2.6
1	D	150	PRO	2.5
1	E	148	HIS	2.5
1	A	267	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	2	SER	2.4
1	J	10	TYR	2.4
1	C	151	HIS	2.4
1	I	2	SER	2.4
1	A	2	SER	2.4
1	H	42	LYS	2.4
1	G	151	HIS	2.3
1	I	148	HIS	2.3
1	E	150	PRO	2.3
1	I	150	PRO	2.2
1	G	148	HIS	2.2
1	F	151	HIS	2.1
1	H	264	TYR	2.1
1	B	148	HIS	2.1
1	L	382	GLU	2.1
1	G	42	LYS	2.1
1	G	126	LYS	2.1
1	H	151	HIS	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	D	504	7/7	0.59	0.28	52,54,57,58	7
3	PEG	A	504	7/7	0.64	0.27	58,61,62,62	7
2	EDO	D	502	4/4	0.66	0.27	63,64,64,64	0
8	MG	E	602	1/1	0.67	0.30	50,50,50,50	1
3	PEG	G	604	7/7	0.69	0.23	41,42,42,42	7

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	J	803	4/4	0.71	0.18	59,59,59,60	0
2	EDO	I	502	4/4	0.72	0.19	52,52,53,54	4
3	PEG	G	602	6/7	0.72	0.28	54,56,56,56	6
3	PEG	J	801	7/7	0.75	0.27	51,54,55,55	7
2	EDO	L	501	4/4	0.76	0.20	42,42,42,42	4
7	MOE	F	507	5/5	0.76	0.19	57,58,59,59	0
3	PEG	G	601	7/7	0.76	0.20	54,55,56,56	7
3	PEG	D	503	7/7	0.77	0.20	56,57,58,58	7
7	MOE	B	503	5/5	0.78	0.20	47,48,49,50	0
2	EDO	G	605	4/4	0.79	0.30	62,62,62,62	4
2	EDO	F	501	4/4	0.79	0.13	42,44,44,44	0
2	EDO	H	601	4/4	0.80	0.15	59,59,60,60	0
3	PEG	A	502	7/7	0.80	0.27	49,49,50,50	7
4	GOL	A	507	6/6	0.81	0.23	74,75,75,75	0
2	EDO	I	501	4/4	0.81	0.23	48,49,50,50	4
9	PG4	D	501	13/13	0.81	0.26	40,43,48,49	13
9	PG4	D	505	13/13	0.83	0.20	27,31,34,34	13
2	EDO	B	504	4/4	0.84	0.17	57,57,58,59	0
2	EDO	C	603	4/4	0.84	0.27	43,44,45,46	0
2	EDO	A	501	4/4	0.84	0.21	45,46,48,49	0
2	EDO	B	502	4/4	0.84	0.15	42,42,42,43	4
2	EDO	F	502	4/4	0.84	0.18	34,35,35,35	0
2	EDO	F	504	4/4	0.85	0.17	56,56,57,57	0
3	PEG	K	501	7/7	0.85	0.18	32,35,37,37	7
2	EDO	J	802	4/4	0.88	0.20	56,56,57,57	0
2	EDO	L	502	4/4	0.88	0.19	55,56,56,57	4
3	PEG	G	603	7/7	0.88	0.23	53,54,55,55	7
2	EDO	A	503	4/4	0.88	0.16	54,55,55,55	4
2	EDO	L	503	4/4	0.89	0.17	51,51,51,52	4
2	EDO	F	503	4/4	0.90	0.14	53,53,54,54	0
2	EDO	A	506	4/4	0.90	0.15	37,40,41,41	0
2	EDO	I	505	4/4	0.90	0.13	47,48,48,48	0
2	EDO	A	505	4/4	0.91	0.12	36,38,40,42	0
2	EDO	C	602	4/4	0.92	0.14	23,24,25,26	4
2	EDO	B	501	4/4	0.92	0.12	32,34,35,37	0
8	MG	B	505	1/1	0.92	0.41	49,49,49,49	1
5	ATP	H	603	31/31	0.93	0.12	45,56,76,76	0
8	MG	K	502	1/1	0.94	0.17	31,31,31,31	1
2	EDO	C	601	4/4	0.94	0.15	53,53,54,55	0
5	ATP	J	805	31/31	0.94	0.11	39,46,65,66	0
5	ATP	E	604	31/31	0.95	0.10	42,46,66,66	0
5	ATP	G	607	31/31	0.95	0.10	43,50,67,68	0

Continued on next page...

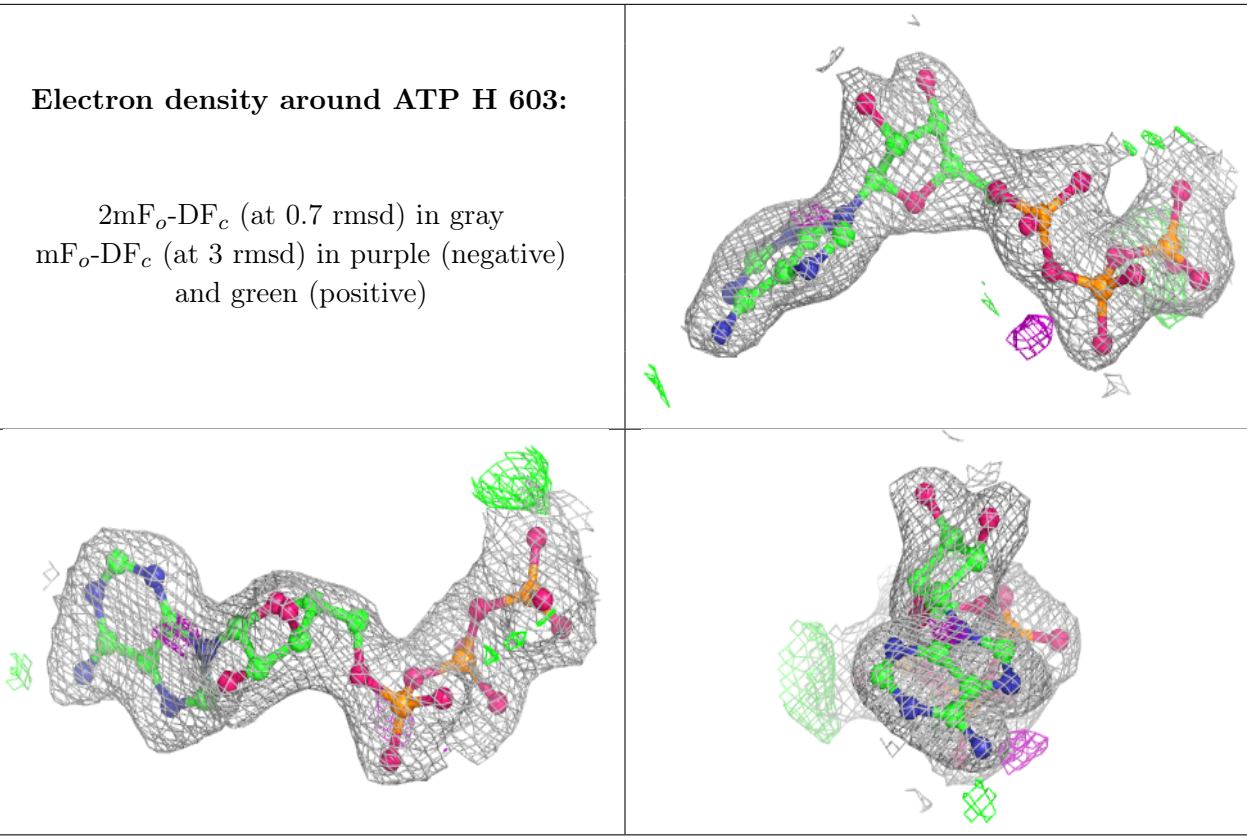
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ATP	B	506	31/31	0.95	0.11	41,45,63,64	0
5	ATP	C	604	31/31	0.95	0.10	45,48,65,65	0
5	ATP	L	505	31/31	0.95	0.10	37,42,61,61	0
5	ATP	D	506	31/31	0.95	0.12	35,40,62,63	0
5	ATP	I	504	31/31	0.96	0.09	40,44,62,63	0
5	ATP	F	506	31/31	0.96	0.10	40,45,66,68	0
5	ATP	K	504	31/31	0.96	0.10	39,44,65,67	0
2	EDO	E	601	4/4	0.96	0.16	75,75,75,75	0
6	AKG	I	503	10/10	0.96	0.10	28,33,38,39	0
5	ATP	A	508	31/31	0.96	0.10	39,41,61,61	0
6	AKG	E	603	10/10	0.97	0.10	27,31,35,36	0
6	AKG	F	505	10/10	0.97	0.10	32,33,34,36	0
6	AKG	H	602	10/10	0.97	0.13	33,34,36,37	0
6	AKG	B	507	10/10	0.97	0.10	28,30,34,34	0
6	AKG	K	503	10/10	0.97	0.10	31,34,37,38	0
6	AKG	C	605	10/10	0.97	0.09	30,30,32,32	0
6	AKG	J	804	10/10	0.98	0.10	27,29,30,31	0
6	AKG	G	606	10/10	0.98	0.10	29,31,34,35	0
6	AKG	L	504	10/10	0.98	0.10	31,32,32,33	0
6	AKG	A	509	10/10	0.98	0.10	31,32,33,34	0
6	AKG	D	507	10/10	0.98	0.09	32,34,36,37	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.

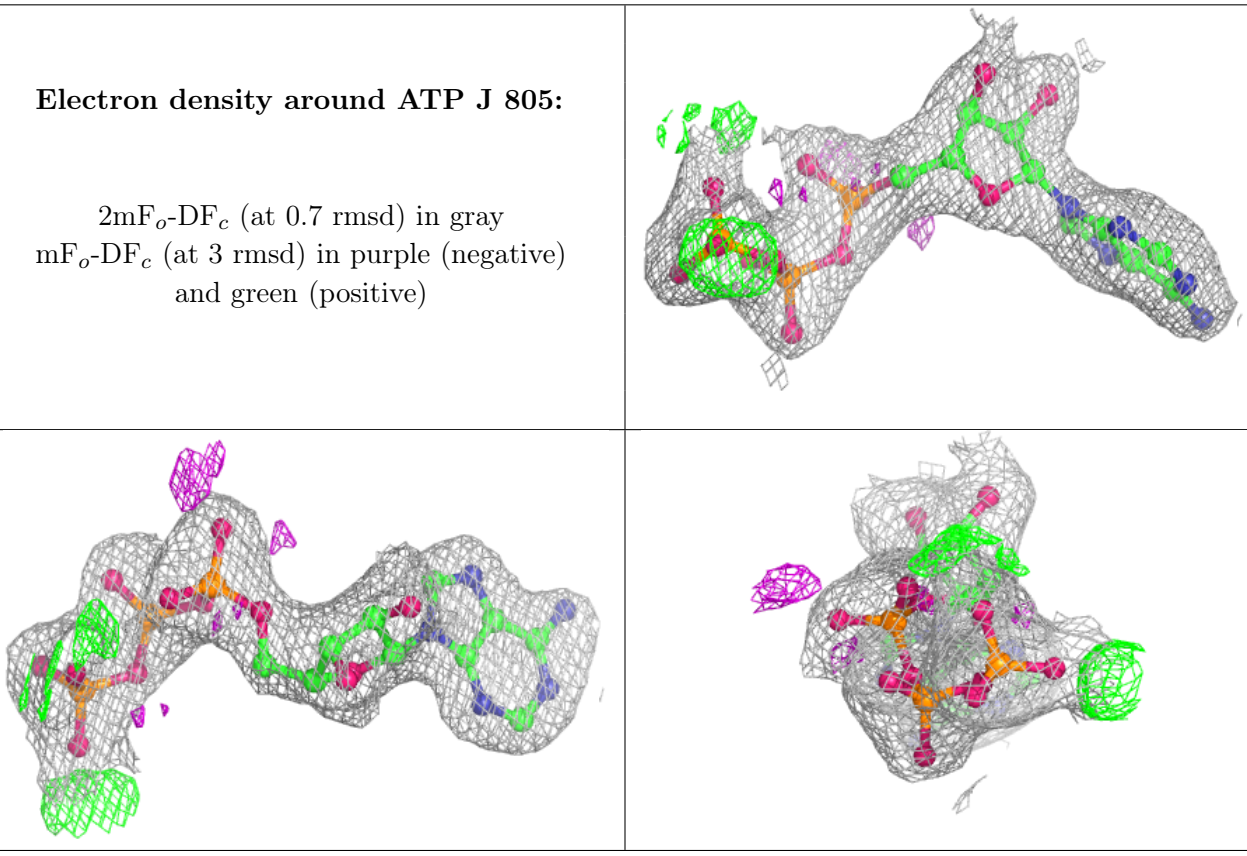
Electron density around ATP H 603:

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



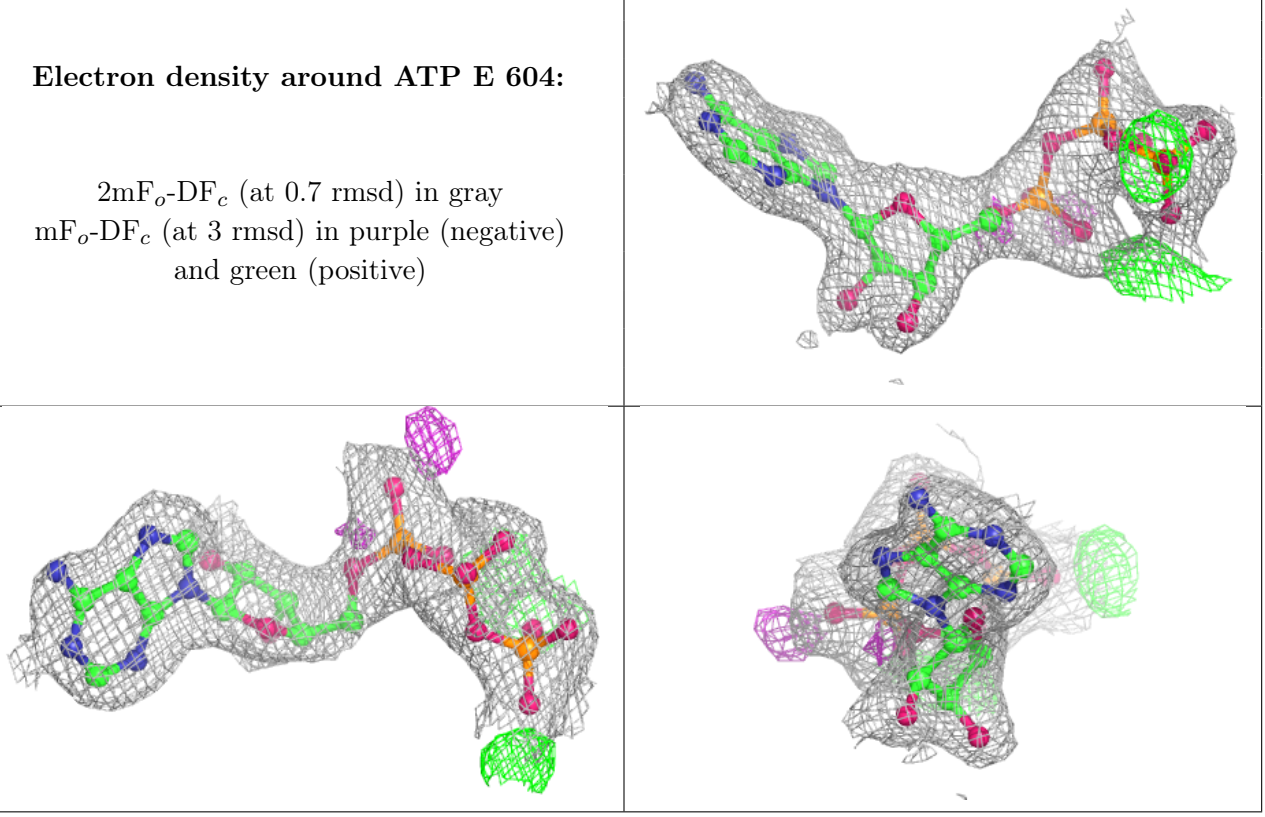
Electron density around ATP J 805:

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



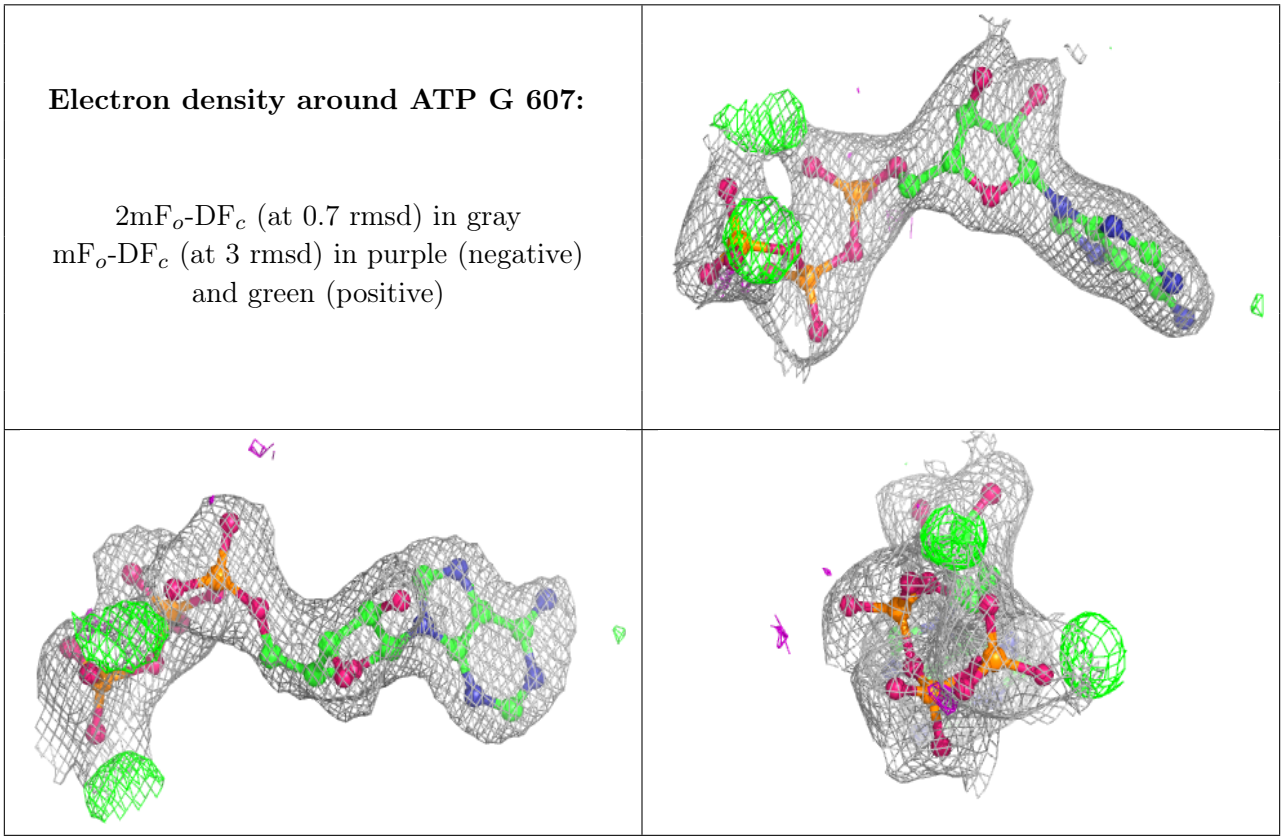
Electron density around ATP E 604:

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



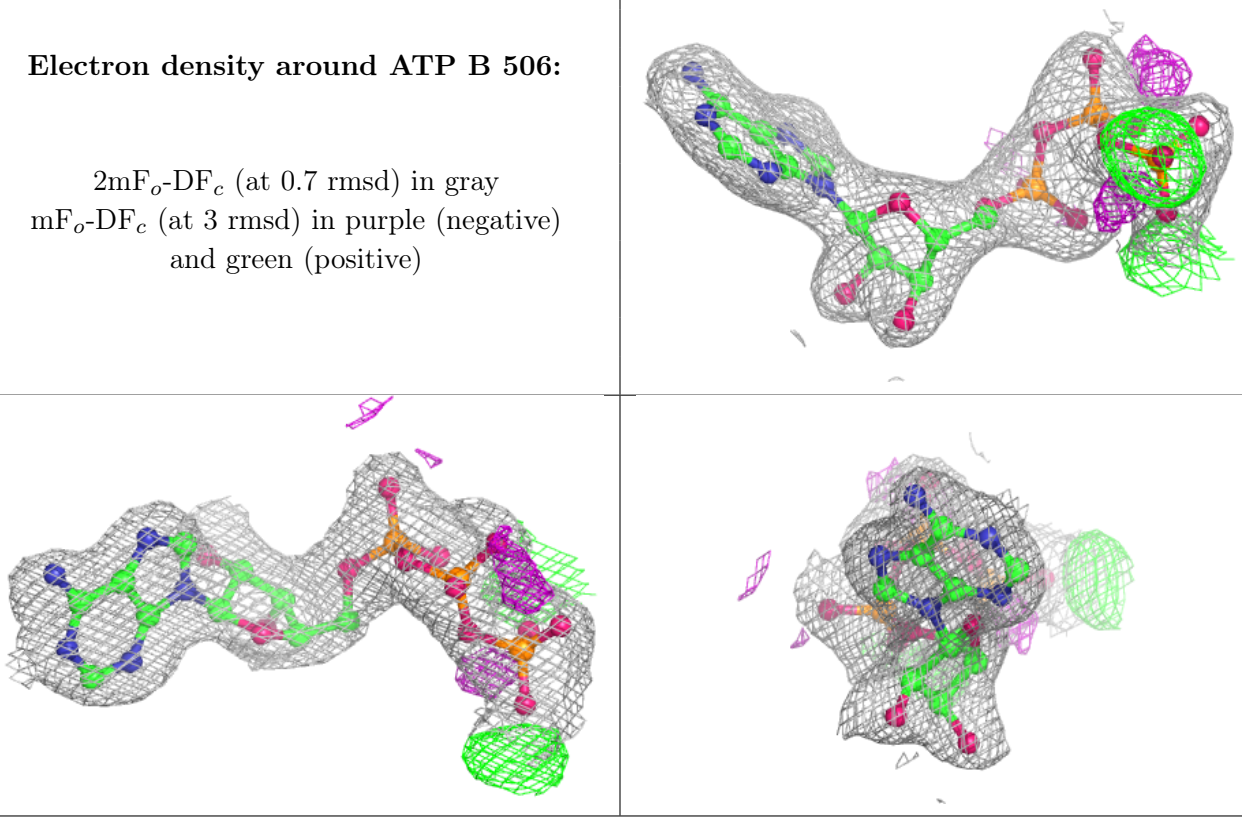
Electron density around ATP G 607:

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



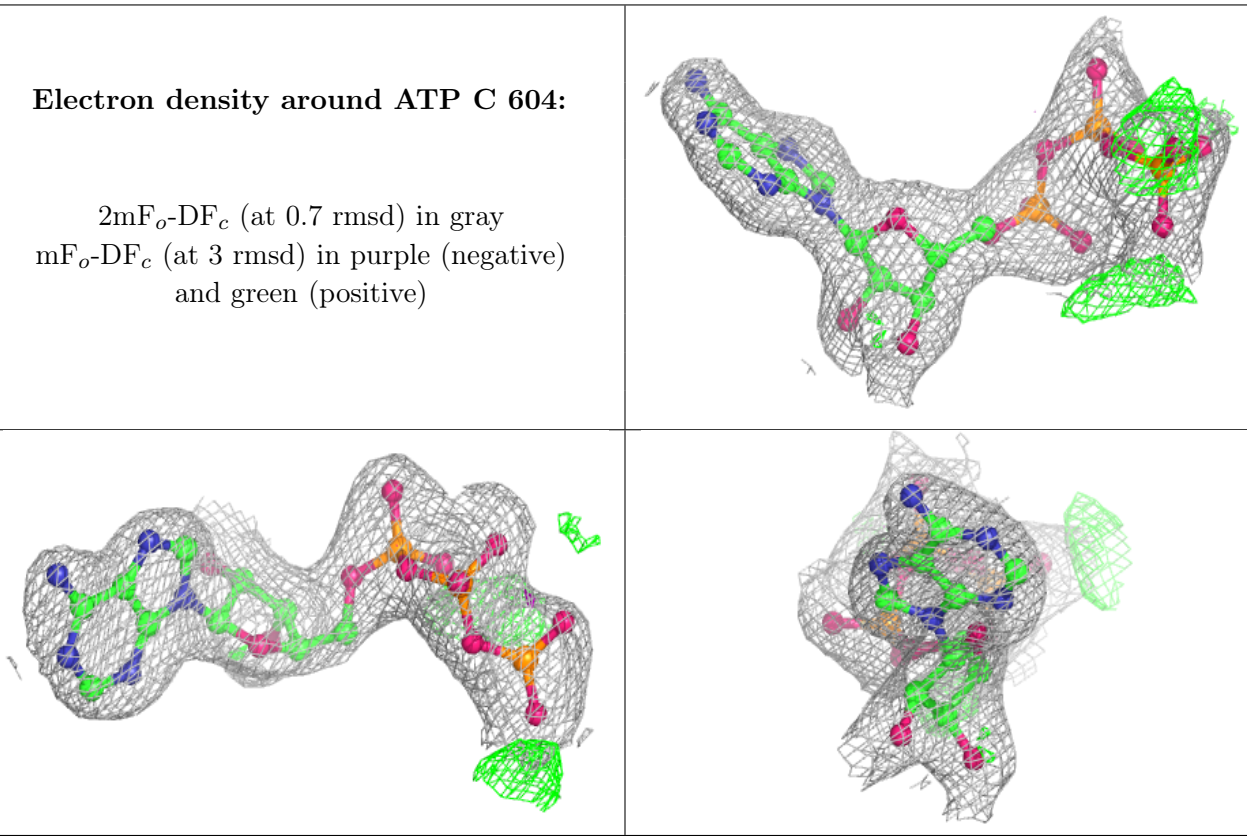
Electron density around ATP B 506:

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



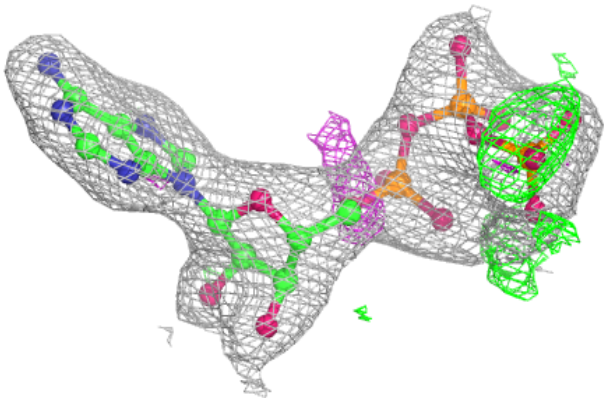
Electron density around ATP C 604:

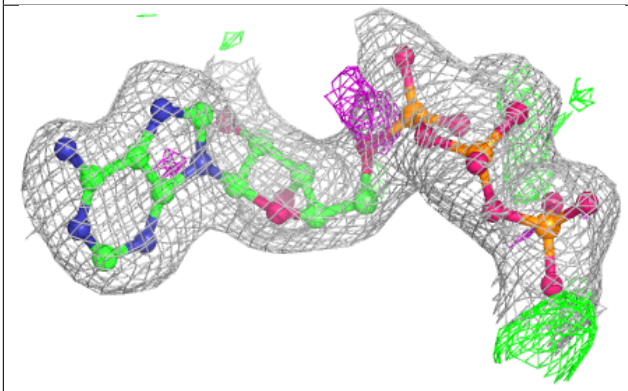
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

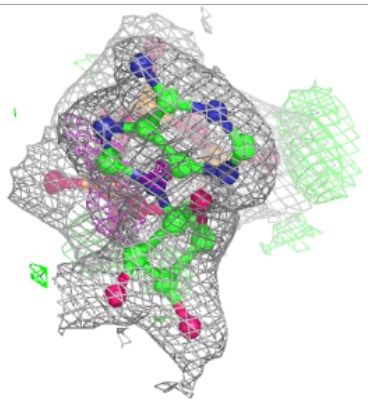


Electron density around ATP L 505:

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

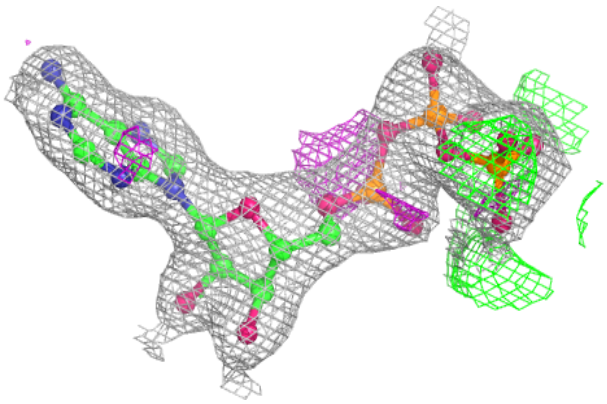


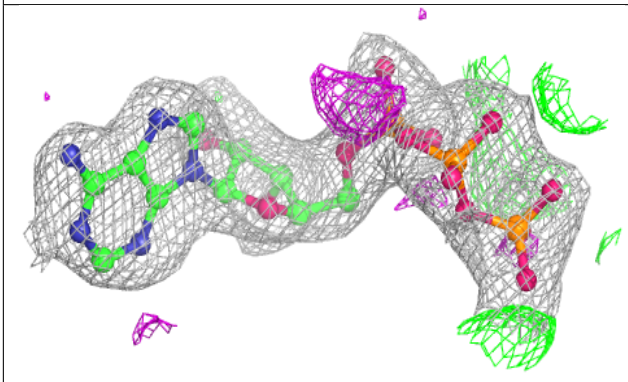


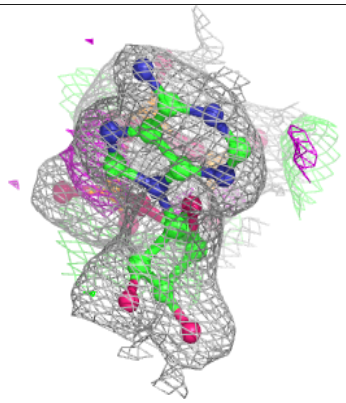


Electron density around ATP D 506:

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

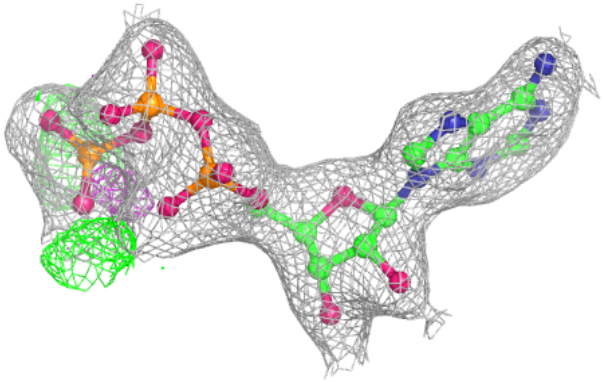


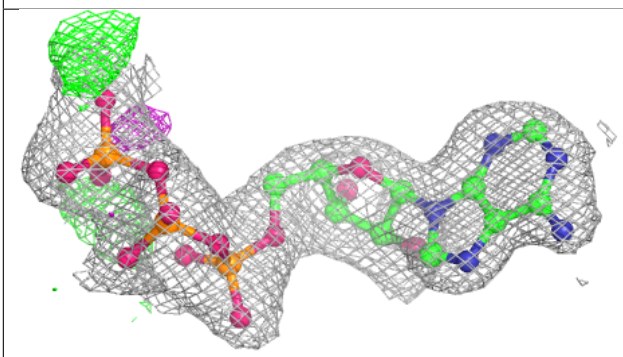


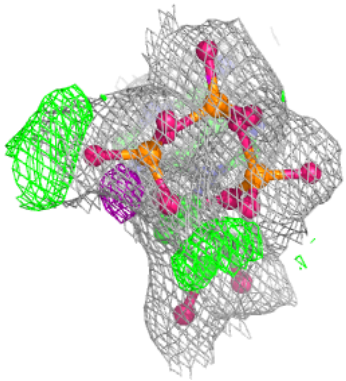


Electron density around ATP I 504:

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

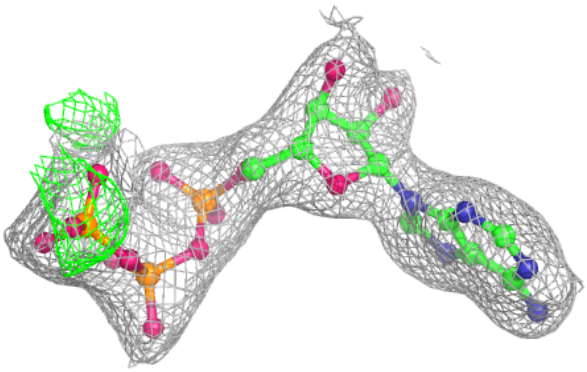


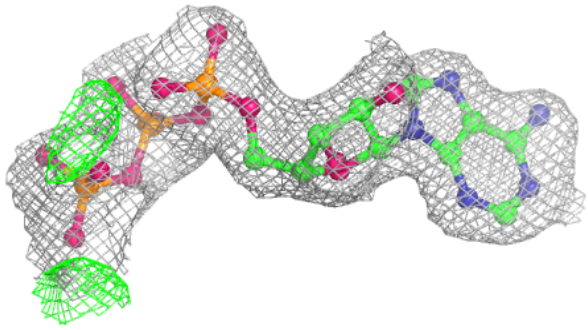


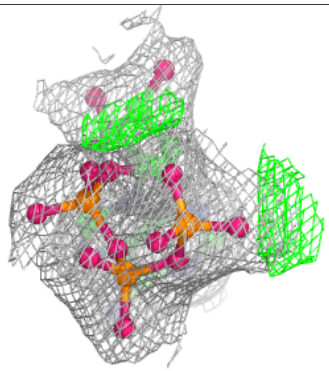


Electron density around ATP F 506:

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

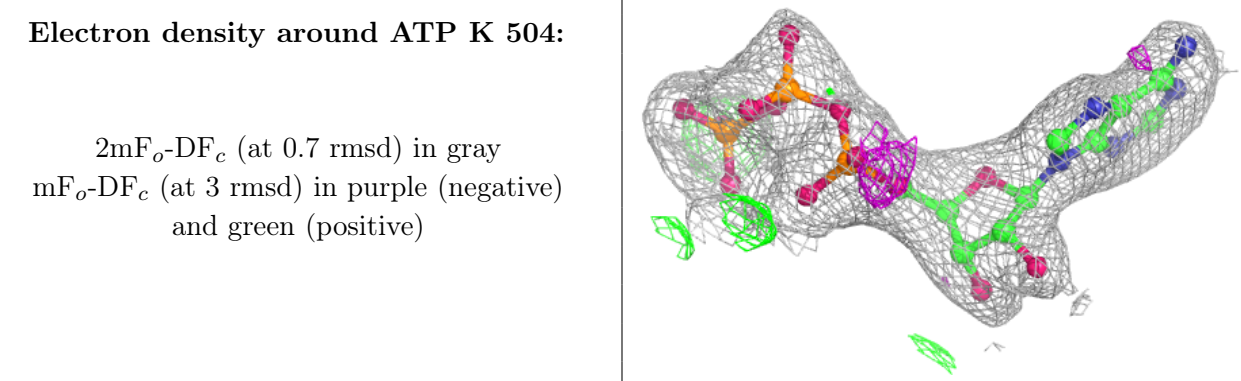


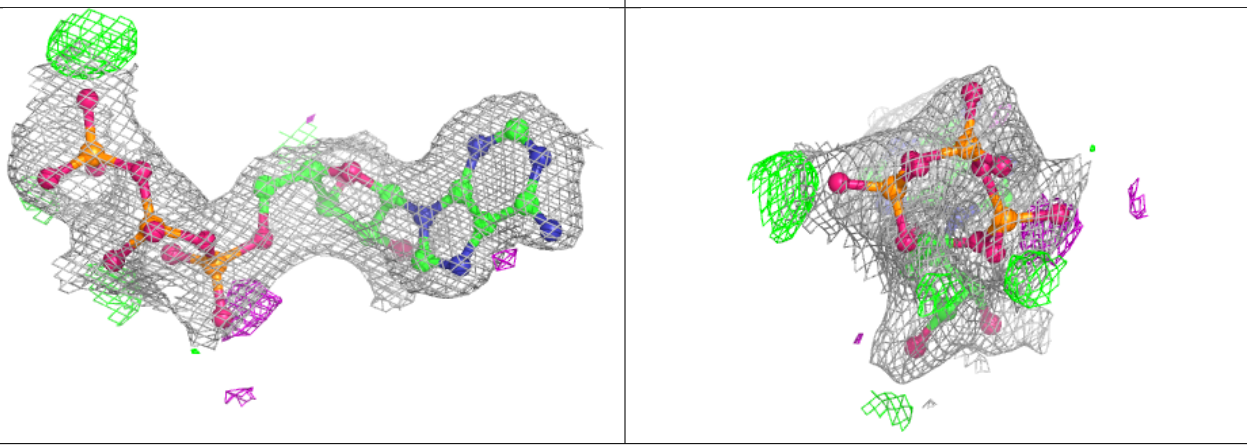




Electron density around ATP K 504:

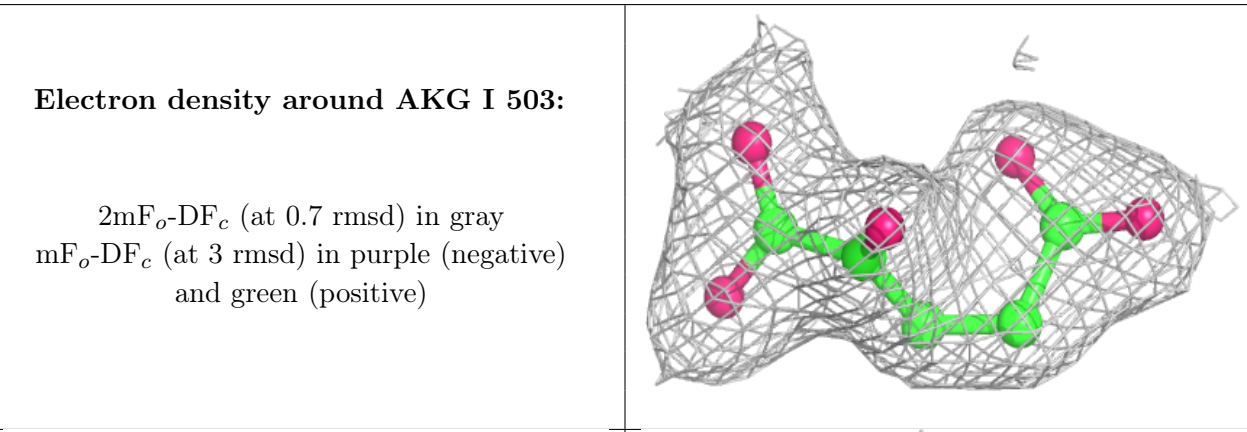
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

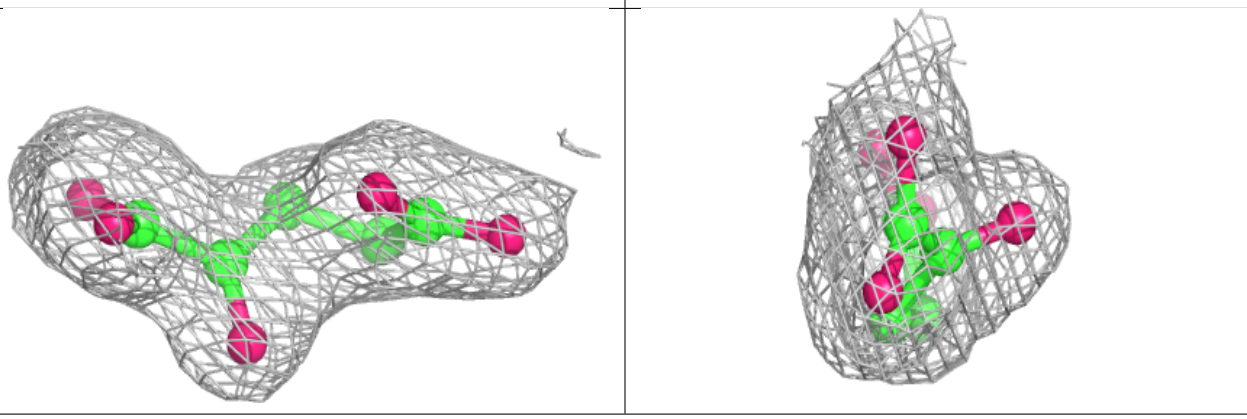




Electron density around AKG I 503:

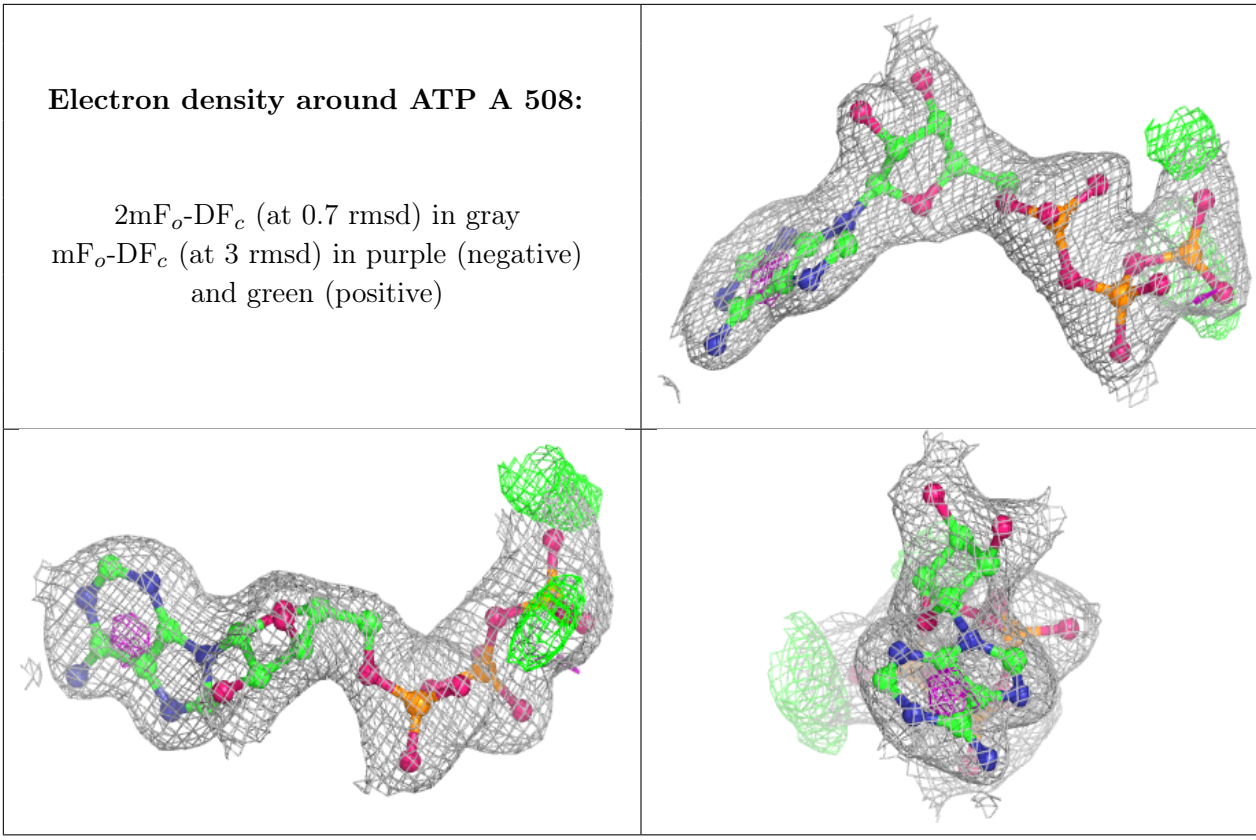
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





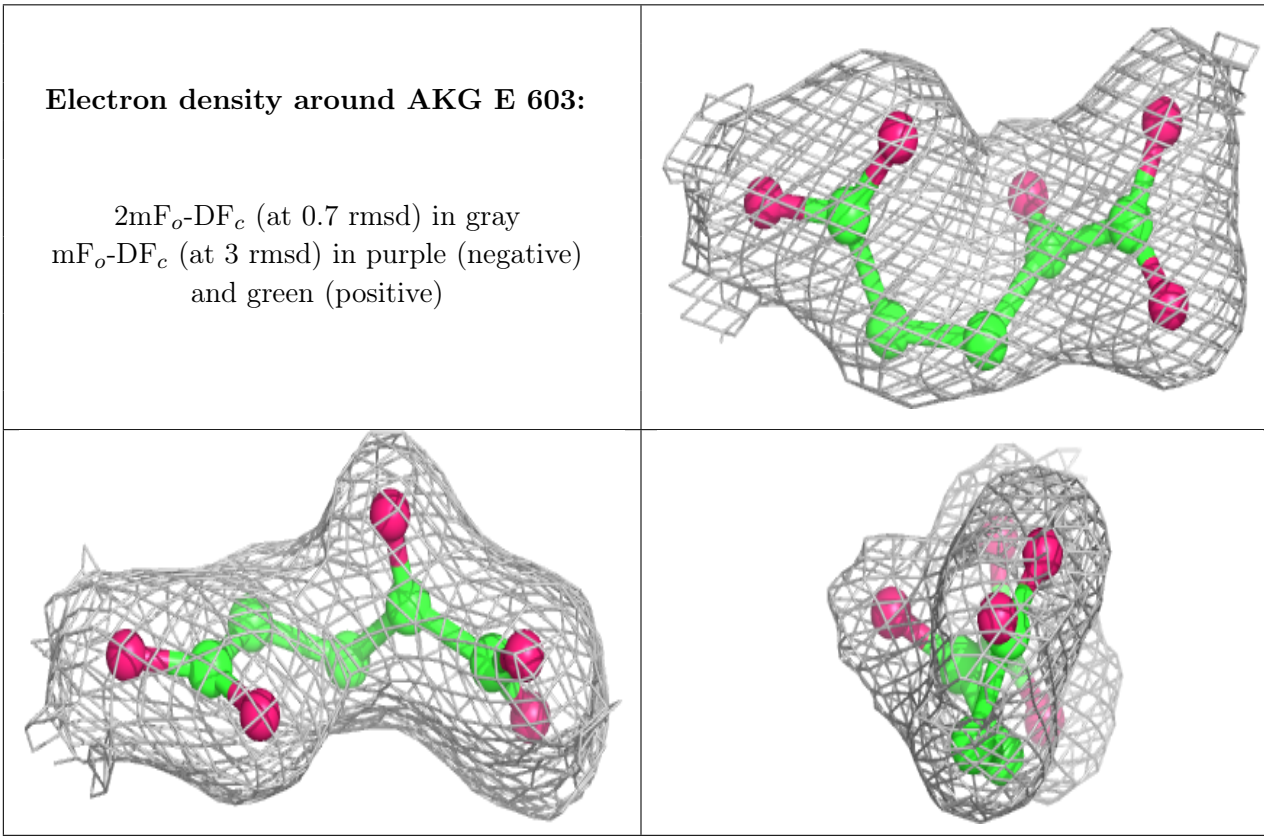
Electron density around ATP A 508:

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



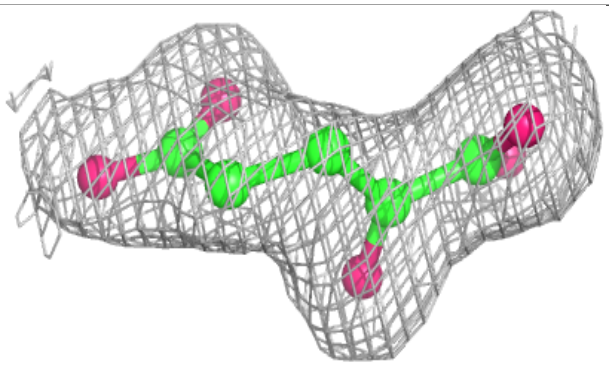
Electron density around AKG E 603:

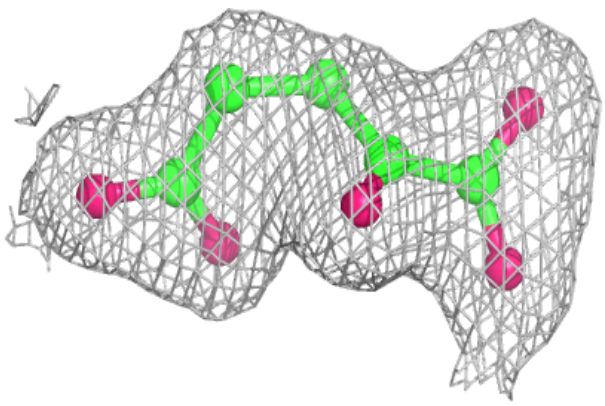
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

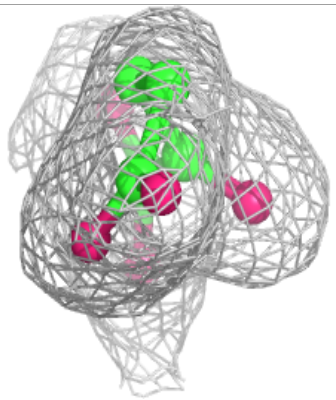


Electron density around AKG F 505:

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

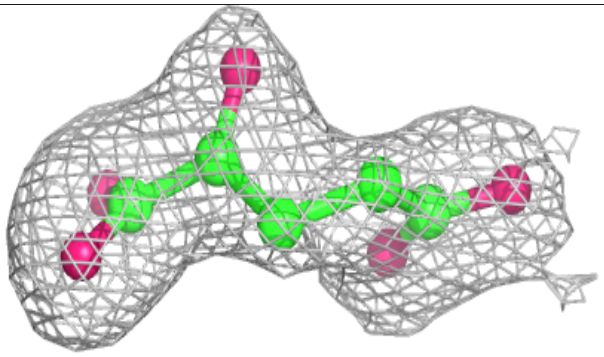


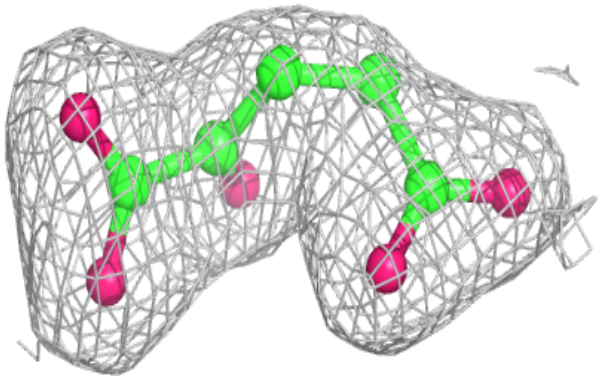


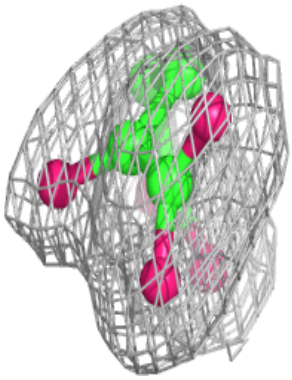


Electron density around AKG H 602:

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

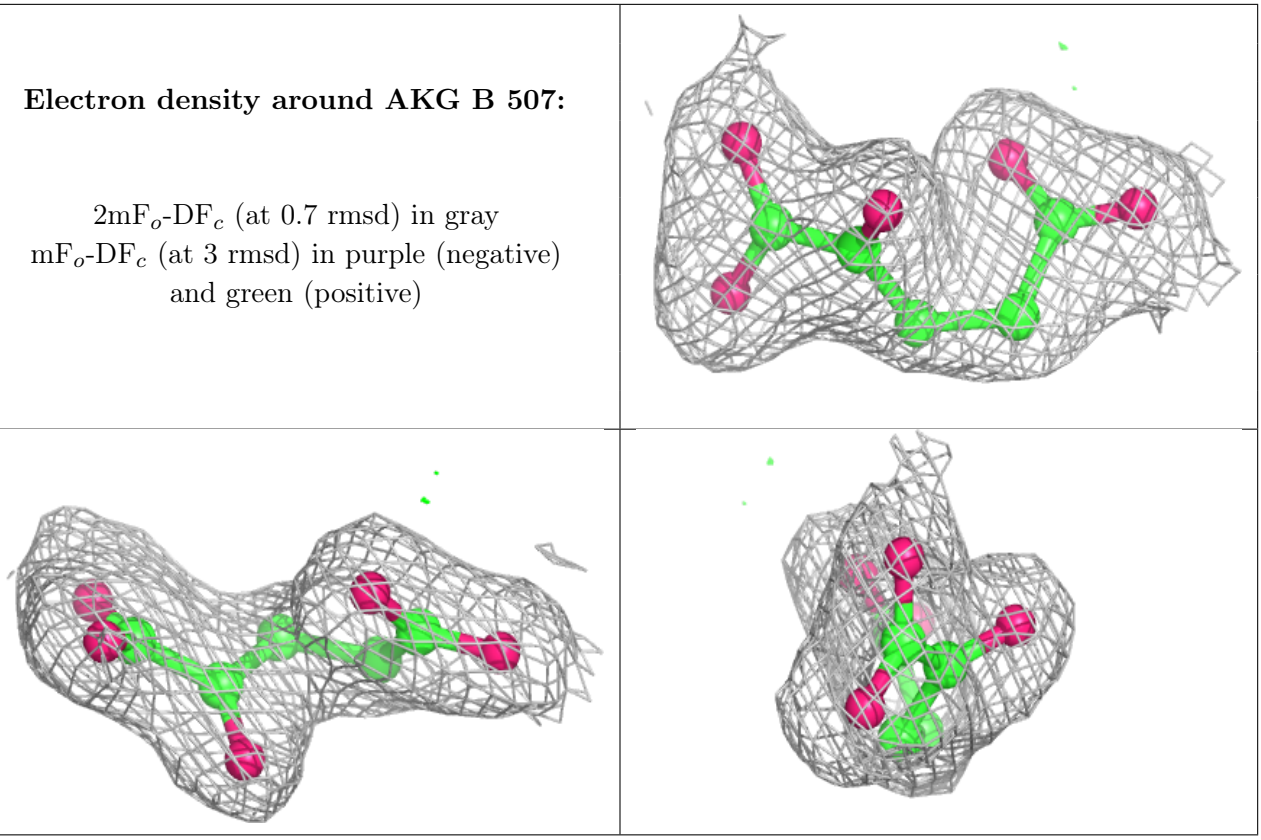






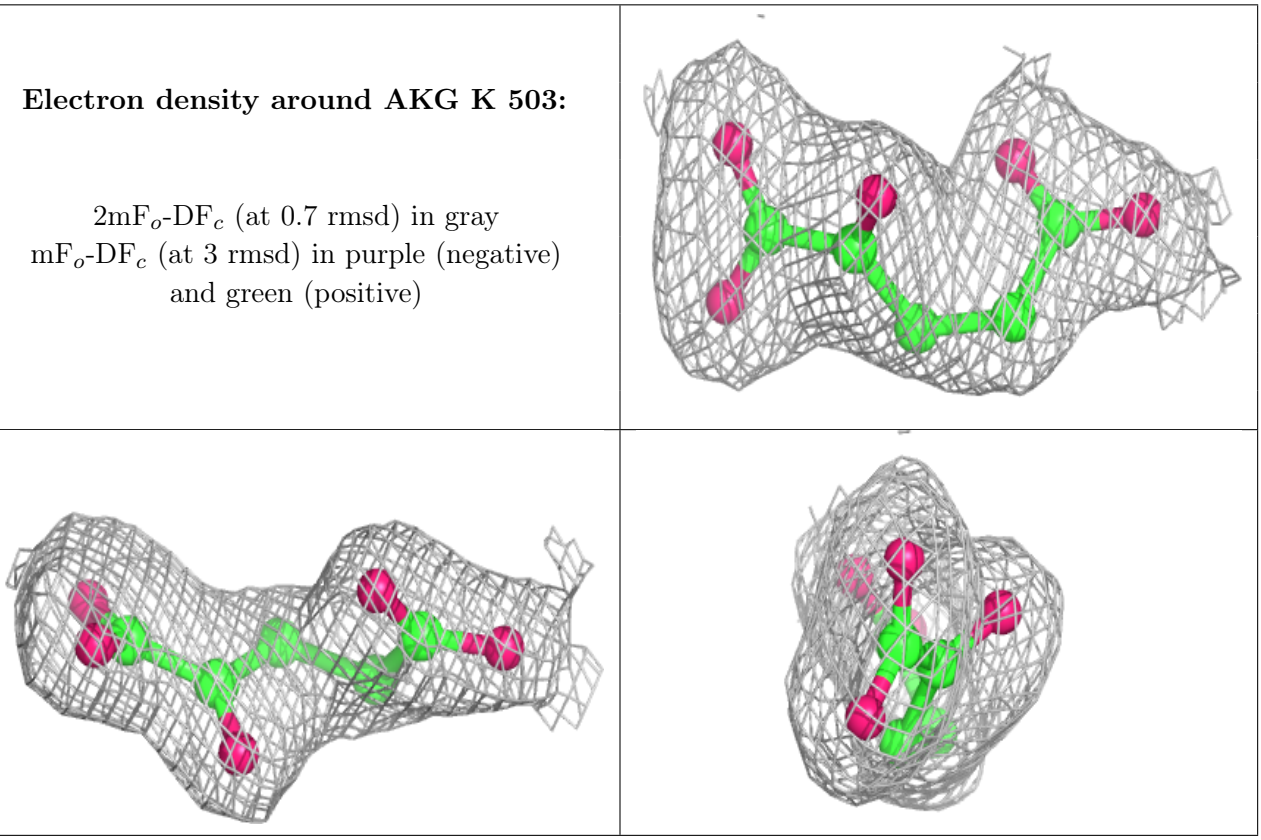
Electron density around AKG B 507:

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



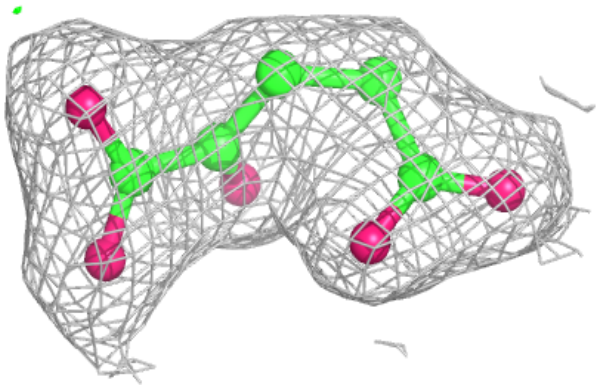
Electron density around AKG K 503:

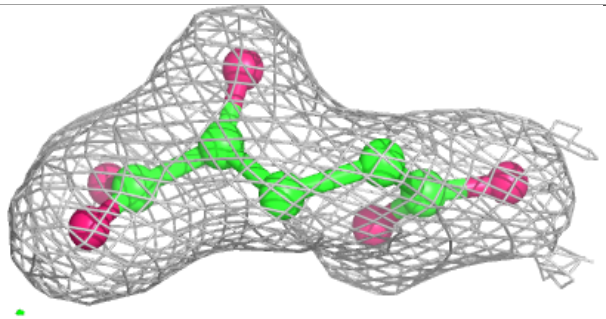
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

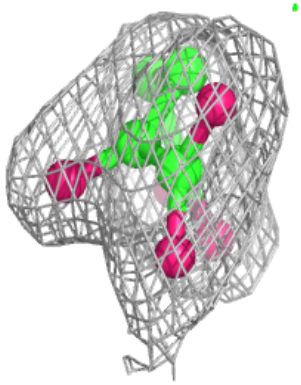


Electron density around AKG C 605:

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

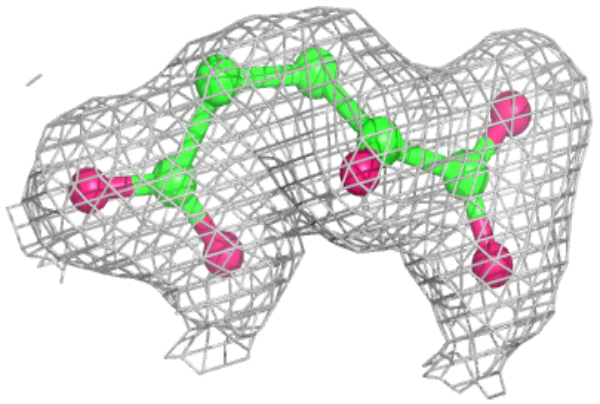


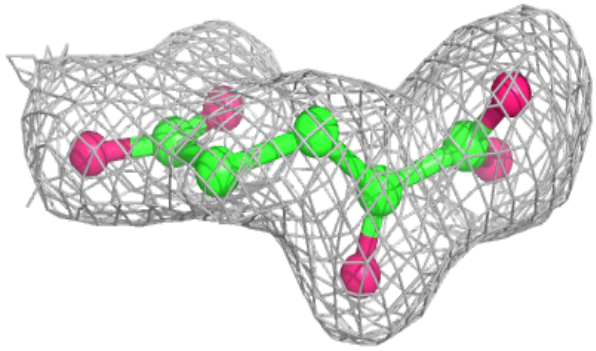


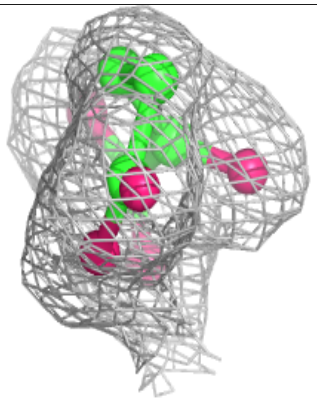


Electron density around AKG J 804:

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

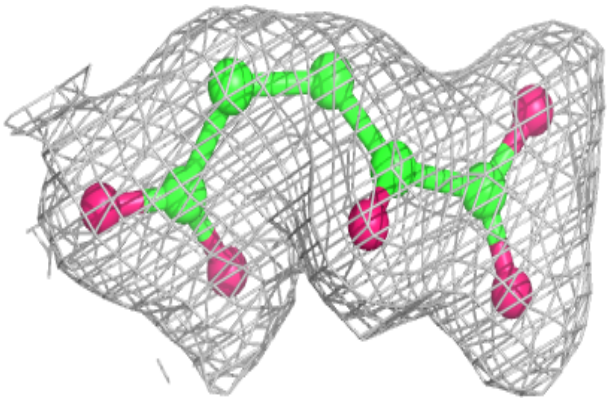


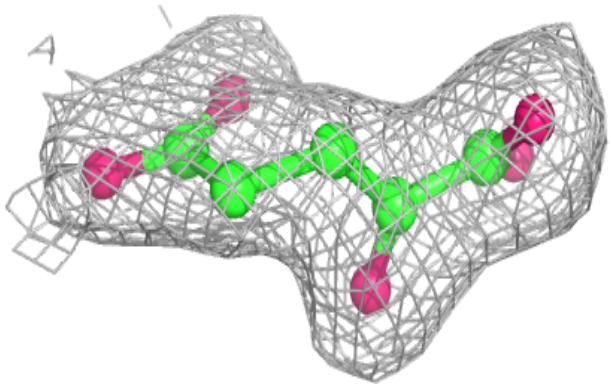


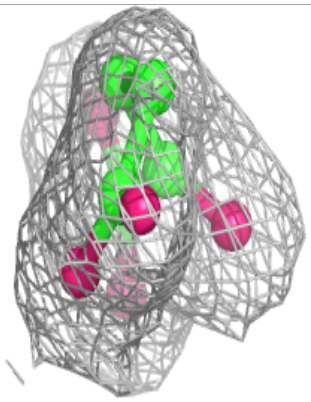


Electron density around AKG G 606:

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

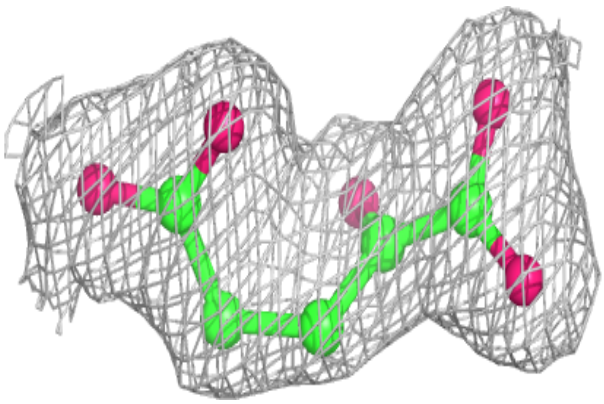


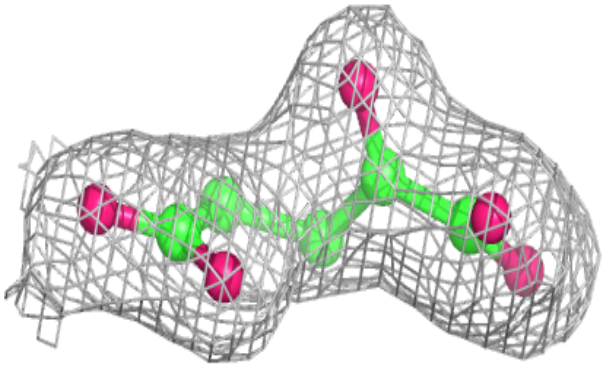


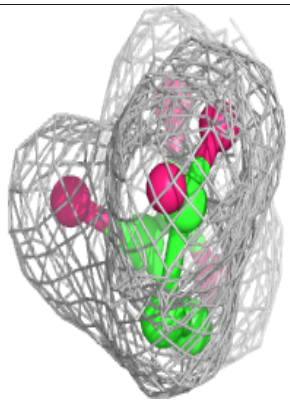


Electron density around AKG L 504:

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

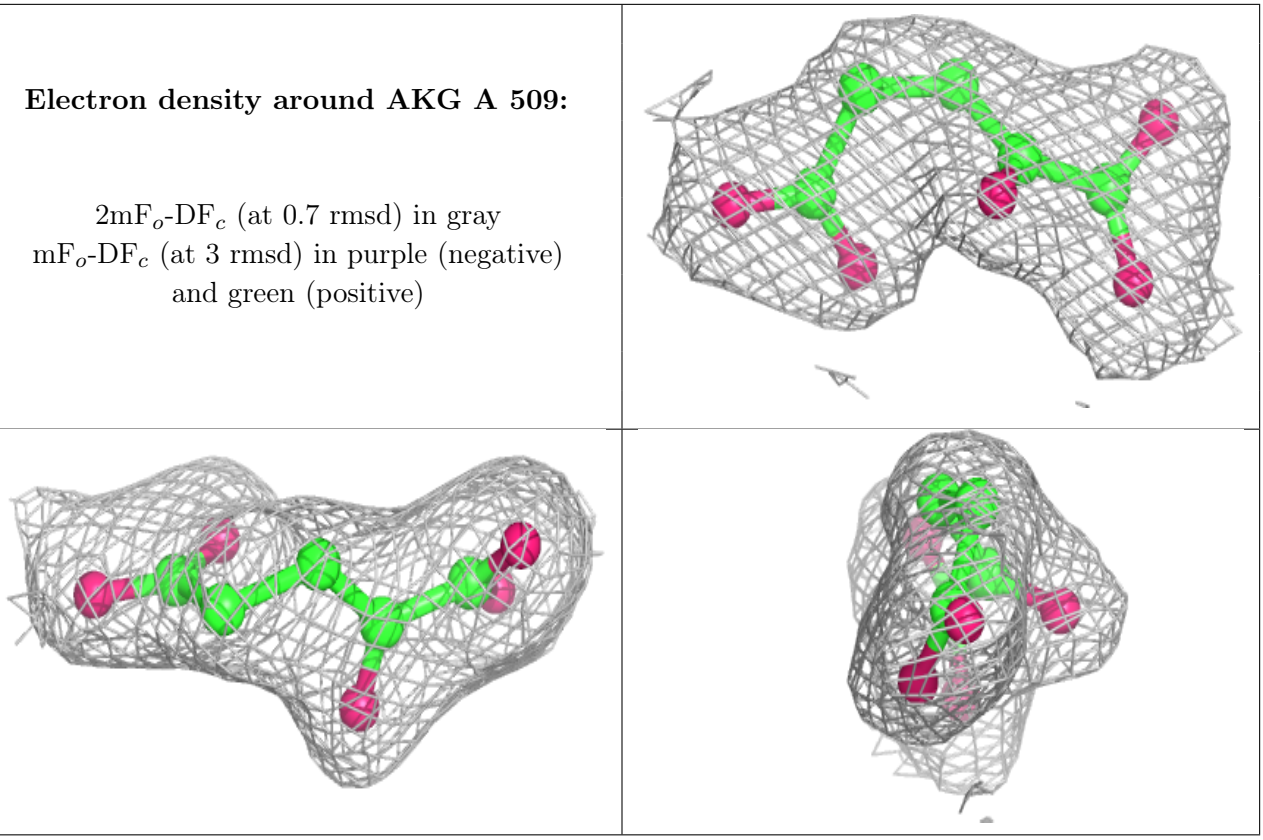






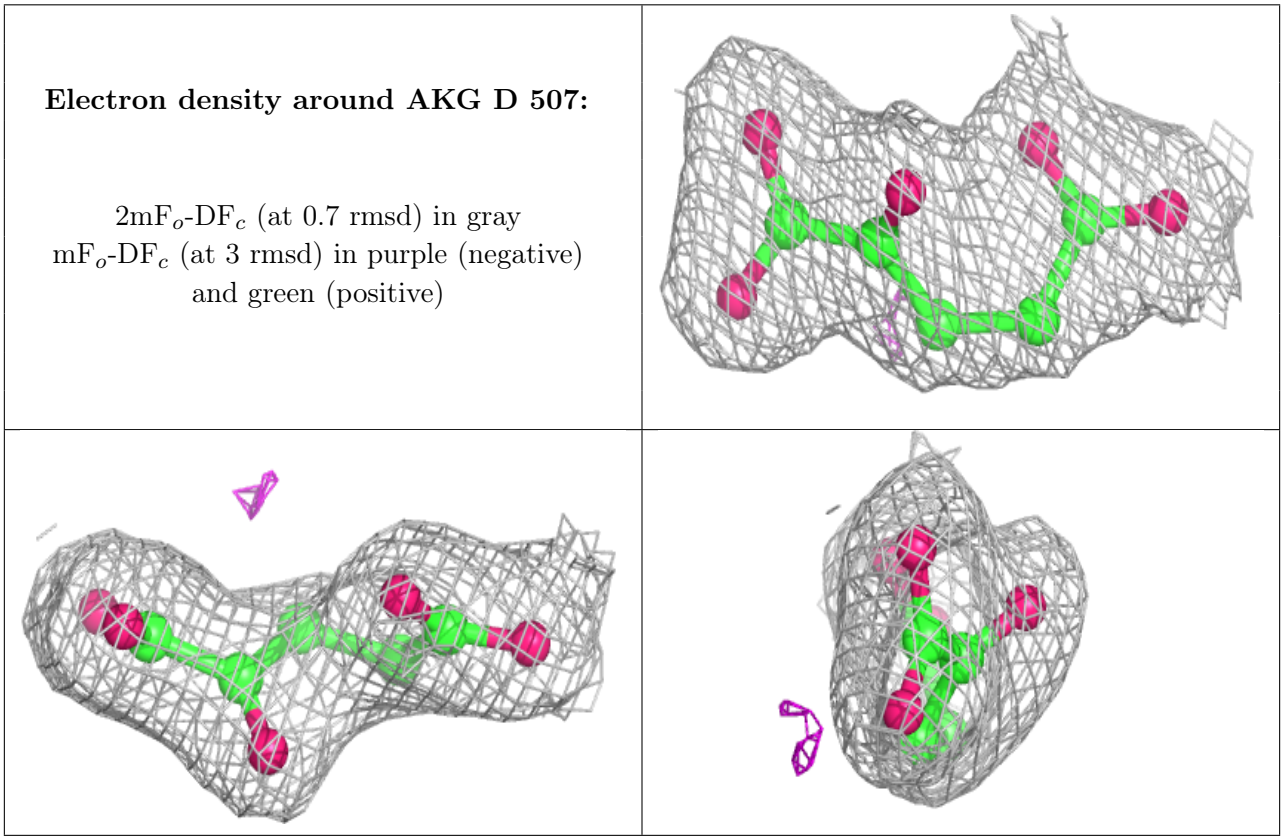
Electron density around AKG A 509:

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



Electron density around AKG D 507:

$2mF_o$-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.