Full wwPDB X-ray Structure Validation Report (i)

May 21, 2025 – 12:35 PM JST

PDB ID	:	8XHQ / pdb_00008xhq
Title	:	The complex structure of SoBcmC and its natural substrate
Authors	:	Wu, L.; Tang, G.L.; Zhou, J.H.
Deposited on	:	2023-12-18
Resolution	:	1.90 Å(reported)

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

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

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

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

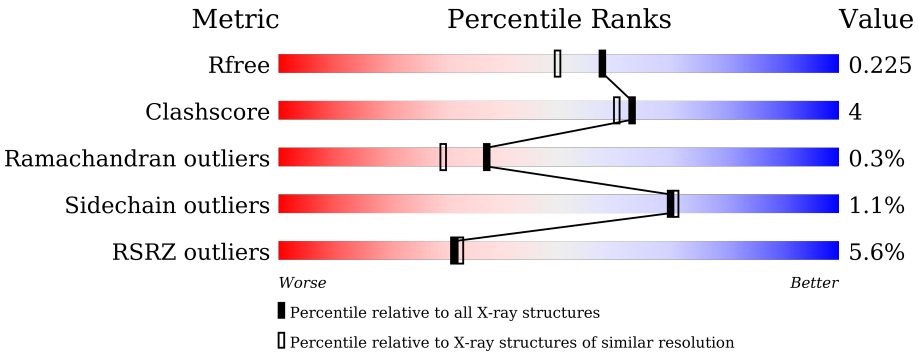
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	311	3% 88% 5% 7%
1	B	311	2% 85% 8% 7%
1	C	311	10% 82% 10% 7%
1	D	311	6% 81% 10% • 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	D	403	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9766 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.

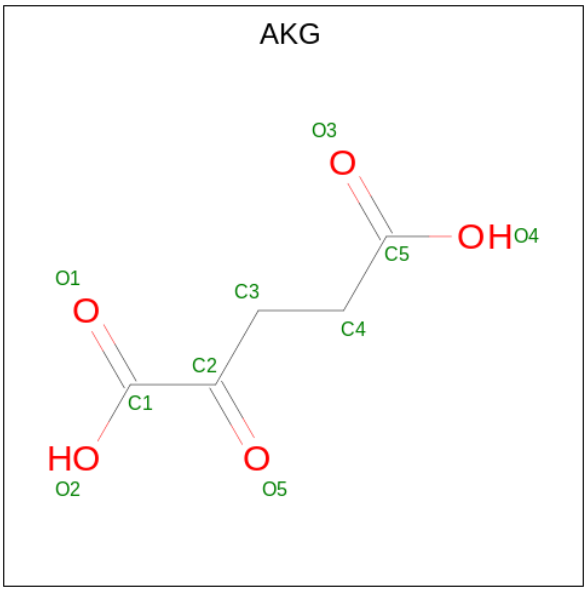
- Molecule 1 is a protein called Fe/2OG dependent dioxigenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	289	Total	C	N	O	S	0	2	0
			2267	1436	393	429	9			
1	A	290	Total	C	N	O	S	0	2	0
			2275	1441	394	431	9			
1	C	288	Total	C	N	O	S	0	2	0
			2266	1433	396	428	9			
1	D	287	Total	C	N	O	S	0	2	0
			2263	1434	392	428	9			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

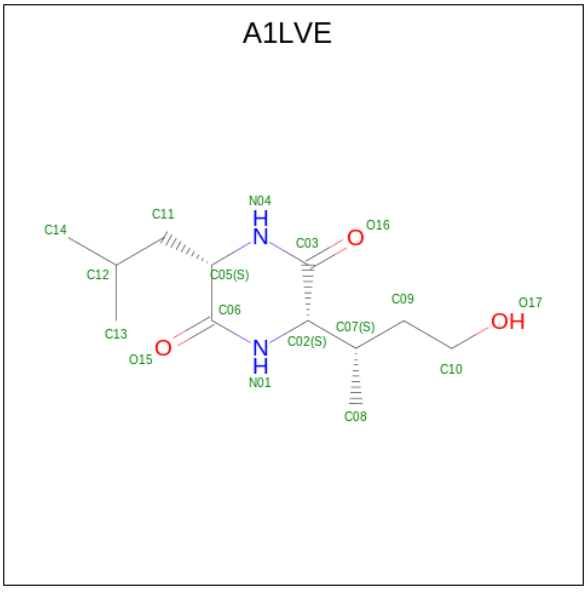
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 10 5 5	0	0
3	A	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0
3	D	1	Total C O 10 5 5	0	0

- Molecule 4 is (3S,6S)-3-(2-methylpropyl)-6-[(2S)-4-oxidanylbutan-2-yl]piperazine-2,5-dione (CCD ID: A1LVE) (formula: $C_{12}H_{22}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			17	12	2	3		
4	A	1	Total	C	N	O	0	0
			17	12	2	3		
4	C	1	Total	C	N	O	0	0
			17	12	2	3		
4	D	1	Total	C	N	O	0	0
			17	12	2	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

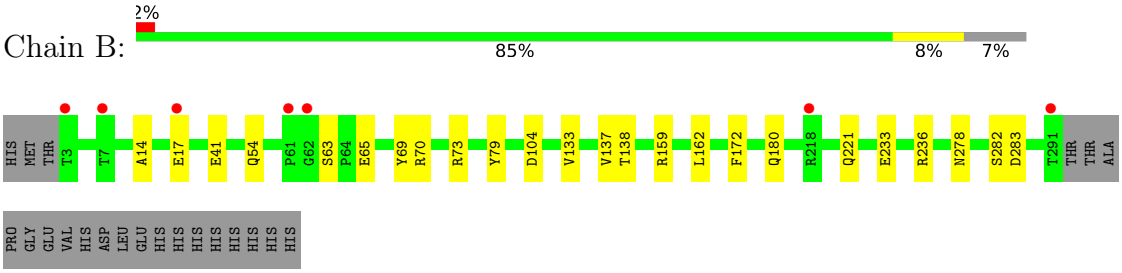
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	183	Total	O	0	0
			183	183		
6	A	185	Total	O	0	0
			185	185		
6	C	122	Total	O	0	0
			122	122		
6	D	92	Total	O	0	0
			92	92		

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.

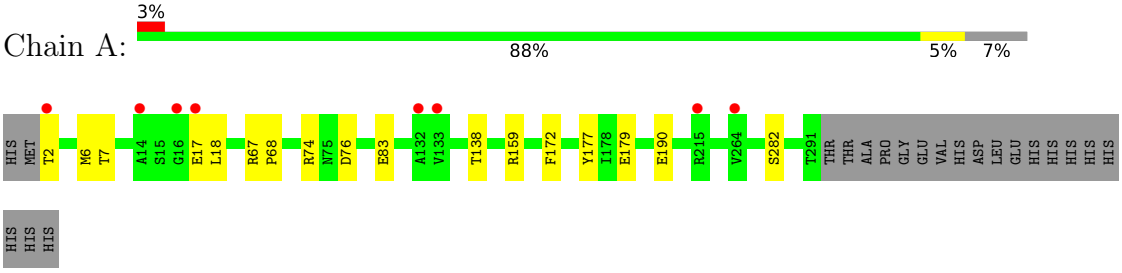
• Molecule 1: Fe/2OG dependent dioxigenase

Chain B:



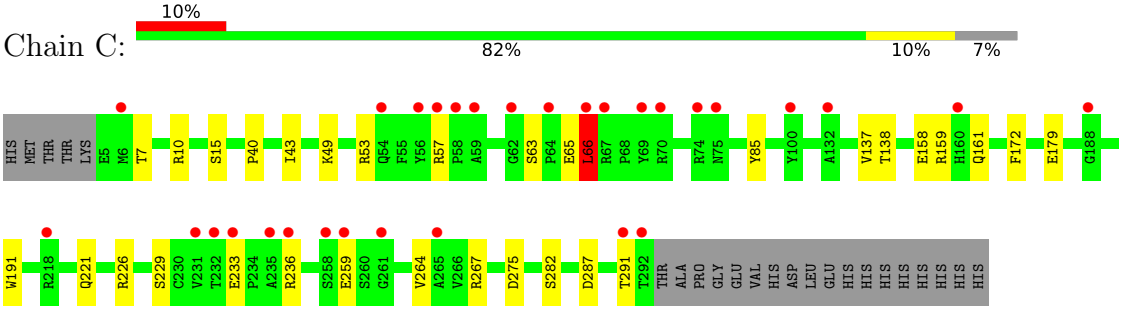
• Molecule 1: Fe/2OG dependent dioxigenase

Chain A:



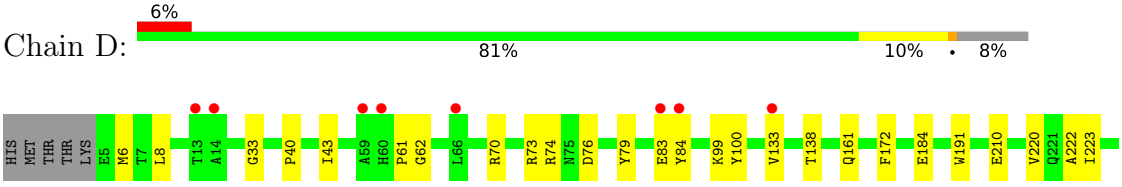
• Molecule 1: Fe/2OG dependent dioxigenase

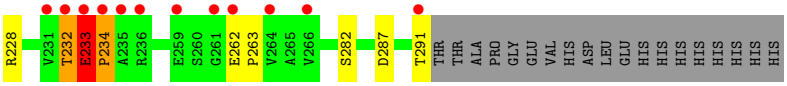
Chain C:



• Molecule 1: Fe/2OG dependent dioxigenase

Chain D:




R228
V231
T232
E233
P234
A235
R236
E259
S260
G261
E262
P263
V264
A265
V266
S282
D287
T291
THR
THR
ALA
PRO
GLY
GLU
VAL
HIS
ASP
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.19Å 142.99Å 85.44Å 90.00° 92.90° 90.00°	Depositor
Resolution (Å)	44.87 – 1.90 44.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.87-1.90) 99.7 (44.87-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.198 , 0.224 0.198 , 0.225	Depositor DCC
R_{free} test set	4794 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9766	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: FE2, A1LVE, AKG, CL

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	0.32	0/2340	0.53	0/3181
1	B	0.34	0/2332	0.52	0/3170
1	C	0.35	0/2325	0.58	1/3160 (0.0%)
1	D	0.30	0/2323	0.55	3/3158 (0.1%)
All	All	0.33	0/9320	0.55	4/12669 (0.0%)

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	66	LEU	CA-CB-CG	6.79	140.08	116.30
1	D	232	THR	CA-C-N	6.50	137.65	121.80
1	D	232	THR	C-N-CA	6.50	137.65	121.80
1	D	233	GLU	N-CA-C	5.18	121.26	109.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	233	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2275	0	2194	13	0
1	B	2267	0	2185	16	0
1	C	2266	0	2177	19	0
1	D	2263	0	2168	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	17	0	0	0	0
4	B	17	0	0	0	0
4	C	17	0	0	0	0
4	D	17	0	0	0	0
5	D	1	0	0	3	0
6	A	185	0	0	5	0
6	B	183	0	0	4	1
6	C	122	0	0	4	0
6	D	92	0	0	1	0
All	All	9766	0	8740	70	1

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 4.

All (70) 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:D:133:VAL:HG21	1:D:263:PRO:HG3	1.57	0.84
1:D:232:THR:O	1:D:234:PRO:HD2	1.85	0.76
1:B:236:ARG:NH2	6:B:503:HOH:O	2.21	0.74
1:B:283:ASP:OD2	6:B:501:HOH:O	2.06	0.72
1:D:61:PRO:O	1:D:70:ARG:NH1	2.24	0.71
1:A:83:GLU:OE1	6:A:501:HOH:O	2.10	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:GLY:HA3	1:D:70:ARG:HH12	1.60	0.66
1:C:287:ASP:HB3	1:C:291:THR:HG22	1.79	0.65
1:C:65:GLU:N	1:C:65:GLU:OE2	2.33	0.61
1:B:180:GLN:OE1	1:B:236:ARG:NH2	2.33	0.61
1:A:67:ARG:NH2	6:A:505:HOH:O	2.32	0.59
1:A:76:ASP:OD1	6:A:502:HOH:O	2.16	0.59
1:D:62:GLY:HA3	1:D:70:ARG:NH1	2.17	0.59
1:D:99:LYS:NZ	1:D:100:TYR:OH	2.34	0.58
1:C:233:GLU:OE1	1:C:236:ARG:NH1	2.37	0.57
1:B:233:GLU:HB3	1:B:236:ARG:HE	1.68	0.57
1:A:74:ARG:NH2	6:A:506:HOH:O	2.35	0.55
1:C:85:TYR:O	1:C:159:ARG:NH1	2.40	0.54
1:A:6:MET:SD	6:A:610:HOH:O	2.59	0.54
1:B:41:GLU:H	1:B:41:GLU:CD	2.16	0.53
1:C:158:GLU:HG2	1:C:159:ARG:HG3	1.90	0.52
1:C:159:ARG:NH1	1:C:161:GLN:OE1	2.42	0.52
1:C:63:SER:OG	1:C:66:LEU:HB3	2.10	0.52
1:D:184:GLU:OE1	1:D:228:ARG:HD3	2.10	0.52
1:D:138:THR:HA	1:D:172:PHE:CZ	2.45	0.52
1:C:49:LYS:HE3	1:C:179:GLU:OE2	2.10	0.52
1:C:221:GLN:HG2	6:C:513:HOH:O	2.10	0.52
1:B:221:GLN:HG2	6:B:507:HOH:O	2.09	0.51
1:C:40:PRO:HD2	1:C:43:ILE:HD12	1.93	0.51
1:D:222:ALA:HA	5:D:403:CL:CL	2.47	0.51
1:D:233:GLU:HG3	1:D:234:PRO:O	2.11	0.51
1:A:138:THR:HA	1:A:172:PHE:CZ	2.47	0.49
1:B:138:THR:HA	1:B:172:PHE:CZ	2.48	0.49
1:B:63:SER:HB2	1:B:65:GLU:OE1	2.13	0.48
1:B:159:ARG:NH2	6:B:506:HOH:O	2.31	0.48
1:B:14:ALA:O	1:B:17:GLU:HG2	2.13	0.47
1:B:54:GLN:OE1	1:B:70:ARG:NE	2.48	0.47
1:A:17:GLU:CD	1:A:18:LEU:H	2.22	0.47
1:C:138:THR:HA	1:C:172:PHE:CZ	2.49	0.47
1:A:2:THR:HG22	1:D:76:ASP:OD1	2.15	0.46
1:D:133:VAL:CG2	1:D:263:PRO:HG3	2.36	0.46
1:C:10[A]:ARG:NE	6:C:507:HOH:O	2.47	0.46
1:D:84[B]:TYR:HA	1:D:161:GLN:NE2	2.30	0.46
1:D:6:MET:HE2	1:D:8:LEU:HD21	1.99	0.46
1:B:278:ASN:HB3	1:D:191:TRP:CZ2	2.52	0.45
1:D:62:GLY:N	6:D:504:HOH:O	2.48	0.45
1:B:69:TYR:OH	1:B:104[A]:ASP:OD2	2.33	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLN:O	1:C:229[B]:SER:HB3	2.17	0.45
1:D:262:GLU:HG3	1:D:263:PRO:HD2	1.99	0.45
1:A:67:ARG:HB3	1:A:68:PRO:HD3	2.00	0.44
1:A:190:GLU:OE2	1:D:74:ARG:NH1	2.50	0.44
1:C:15:SER:O	6:C:501:HOH:O	2.21	0.44
1:D:33:GLY:O	5:D:403:CL:CL	2.73	0.44
1:C:267:ARG:HG3	6:C:519:HOH:O	2.16	0.44
1:A:177:TYR:OH	1:A:179:GLU:OE2	2.26	0.44
1:C:233:GLU:HB3	1:C:236:ARG:HE	1.84	0.43
1:C:191:TRP:CZ2	1:C:226:ARG:HD3	2.54	0.43
1:A:6:MET:HE2	1:A:6:MET:HB3	1.83	0.42
1:D:223:ILE:N	5:D:403:CL:CL	2.75	0.42
1:D:40:PRO:HD2	1:D:43:ILE:HD12	2.01	0.42
1:B:133:VAL:O	1:B:137:VAL:HG22	2.20	0.41
1:D:83[B]:GLU:O	1:D:84[B]:TYR:HB2	2.19	0.41
1:B:73:ARG:HG2	1:B:79:TYR:CZ	2.54	0.41
1:D:210:GLU:HA	1:D:220:VAL:O	2.21	0.41
1:A:177:TYR:CE2	1:A:179:GLU:HG3	2.56	0.41
1:C:267:ARG:NH2	1:C:275:ASP:OD2	2.54	0.41
1:B:162:LEU:HG	1:D:84[A]:TYR:CZ	2.56	0.40
1:D:73:ARG:HG2	1:D:79:TYR:CZ	2.55	0.40
1:D:287:ASP:HB3	1:D:291:THR:HB	2.02	0.40
1:C:53:ARG:O	1:C:57:ARG:NE	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:650:HOH:O	6:B:668:HOH:O[1_655]	2.15	0.05

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	290/311 (93%)	287 (99%)	3 (1%)	0	100	100
1	B	289/311 (93%)	288 (100%)	1 (0%)	0	100	100
1	C	288/311 (93%)	285 (99%)	2 (1%)	1 (0%)	37	29
1	D	287/311 (92%)	280 (98%)	5 (2%)	2 (1%)	19	11
All	All	1154/1244 (93%)	1140 (99%)	11 (1%)	3 (0%)	37	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	233	GLU
1	D	234	PRO
1	C	259	GLU

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	238/255 (93%)	234 (98%)	4 (2%)	56	54
1	B	237/255 (93%)	236 (100%)	1 (0%)	89	90
1	C	236/255 (92%)	231 (98%)	5 (2%)	48	45
1	D	235/255 (92%)	234 (100%)	1 (0%)	89	90
All	All	946/1020 (93%)	935 (99%)	11 (1%)	70	68

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	282	SER
1	A	7[A]	THR
1	A	7[B]	THR
1	A	159	ARG
1	A	282	SER
1	C	7	THR
1	C	66	LEU
1	C	137	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	264	VAL
1	C	282	SER
1	D	282	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	28	GLN
1	A	148	GLN
1	A	160	HIS
1	A	247	ASN
1	C	148	GLN
1	D	28	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	AKG	A	402	2	9,9,9	2.07	1 (11%)	11,11,11	1.67	4 (36%)
3	AKG	B	402	2	9,9,9	1.83	1 (11%)	11,11,11	2.07	5 (45%)
4	A1LVE	A	404	-	17,17,17	3.16	3 (17%)	19,23,23	1.06	1 (5%)
4	A1LVE	D	404	-	17,17,17	3.04	2 (11%)	19,23,23	1.22	1 (5%)
4	A1LVE	C	403	-	17,17,17	3.20	4 (23%)	19,23,23	1.34	3 (15%)
4	A1LVE	B	403	-	17,17,17	3.00	2 (11%)	19,23,23	1.27	2 (10%)
3	AKG	C	402	2	9,9,9	1.98	2 (22%)	11,11,11	1.83	3 (27%)
3	AKG	D	402	2	9,9,9	2.01	3 (33%)	11,11,11	1.73	4 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AKG	A	402	2	-	0/9/9/9	-
3	AKG	B	402	2	-	2/9/9/9	-
4	A1LVE	A	404	-	-	0/11/27/27	0/1/1/1
4	A1LVE	D	404	-	-	0/11/27/27	0/1/1/1
4	A1LVE	C	403	-	-	1/11/27/27	0/1/1/1
4	A1LVE	B	403	-	-	0/11/27/27	0/1/1/1
3	AKG	C	402	2	-	0/9/9/9	-
3	AKG	D	402	2	-	0/9/9/9	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	A1LVE	C06-N01	9.32	1.48	1.33
4	C	403	A1LVE	C03-N04	9.27	1.48	1.33
4	D	404	A1LVE	C06-N01	8.86	1.47	1.33
4	C	403	A1LVE	C06-N01	8.67	1.47	1.33
4	B	403	A1LVE	C06-N01	8.54	1.46	1.33
4	D	404	A1LVE	C03-N04	8.41	1.46	1.33
4	B	403	A1LVE	C03-N04	8.40	1.46	1.33
4	A	404	A1LVE	C03-N04	8.37	1.46	1.33
3	A	402	AKG	C2-C1	-5.57	1.46	1.53
3	D	402	AKG	C2-C1	-5.00	1.46	1.53
3	C	402	AKG	C2-C1	-5.00	1.46	1.53
3	B	402	AKG	C2-C1	-4.53	1.47	1.53
4	A	404	A1LVE	O15-C06	-2.24	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	A1LVE	O16-C03	-2.22	1.19	1.23
3	C	402	AKG	O2-C1	-2.15	1.24	1.30
4	C	403	A1LVE	O15-C06	-2.01	1.19	1.23
3	D	402	AKG	O2-C1	-2.00	1.24	1.30
3	D	402	AKG	O4-C5	-2.00	1.24	1.30

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	AKG	C3-C2-C1	3.29	122.09	115.97
3	C	402	AKG	C3-C2-C1	2.92	121.40	115.97
4	D	404	A1LVE	O16-C03-N04	-2.87	118.84	122.69
4	C	403	A1LVE	O16-C03-N04	-2.82	118.91	122.69
3	C	402	AKG	C4-C3-C2	-2.75	107.85	113.03
3	B	402	AKG	O5-C2-C3	-2.70	115.22	121.20
3	B	402	AKG	C3-C4-C5	-2.64	107.92	113.60
3	A	402	AKG	C4-C3-C2	-2.58	108.17	113.03
3	A	402	AKG	O1-C1-C2	-2.58	118.28	121.72
4	C	403	A1LVE	C07-C02-N01	-2.56	107.18	111.94
3	A	402	AKG	C3-C2-C1	2.51	120.63	115.97
4	B	403	A1LVE	O16-C03-N04	-2.48	119.36	122.69
4	B	403	A1LVE	O15-C06-N01	-2.46	119.39	122.69
4	A	404	A1LVE	O16-C03-N04	-2.41	119.45	122.69
3	D	402	AKG	C3-C2-C1	2.39	120.40	115.97
4	C	403	A1LVE	C02-C03-N04	2.35	121.08	118.19
3	D	402	AKG	C4-C3-C2	-2.31	108.67	113.03
3	C	402	AKG	O2-C1-C2	2.29	120.24	113.97
3	B	402	AKG	O5-C2-C1	2.24	122.68	119.43
3	A	402	AKG	O2-C1-C2	2.23	120.07	113.97
3	D	402	AKG	O5-C2-C1	2.21	122.64	119.43
3	B	402	AKG	O2-C1-C2	2.15	119.85	113.97
3	D	402	AKG	O2-C1-C2	2.13	119.79	113.97

There are no chirality outliers.

All (3) torsion outliers are listed below:

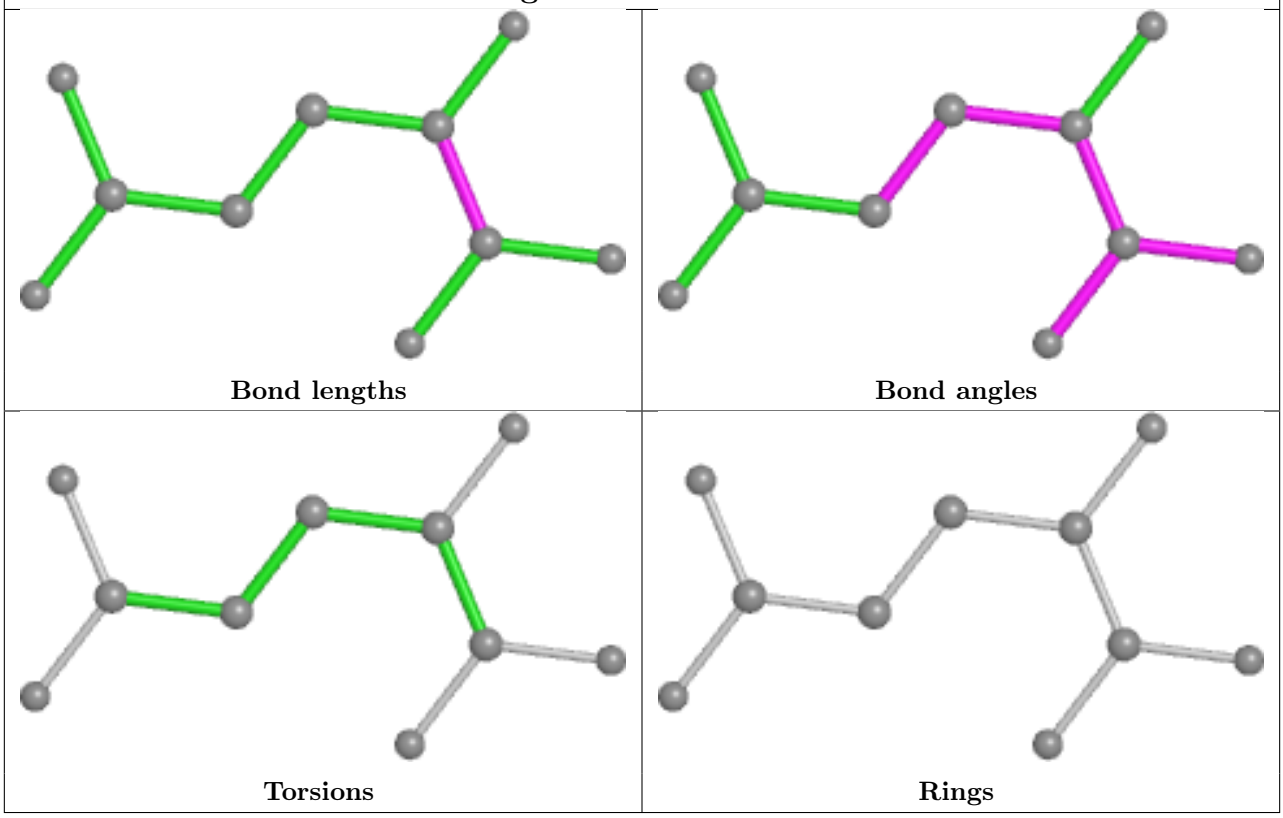
Mol	Chain	Res	Type	Atoms
3	B	402	AKG	C3-C4-C5-O3
3	B	402	AKG	C3-C4-C5-O4
4	C	403	A1LVE	C07-C09-C10-O17

There are no ring outliers.

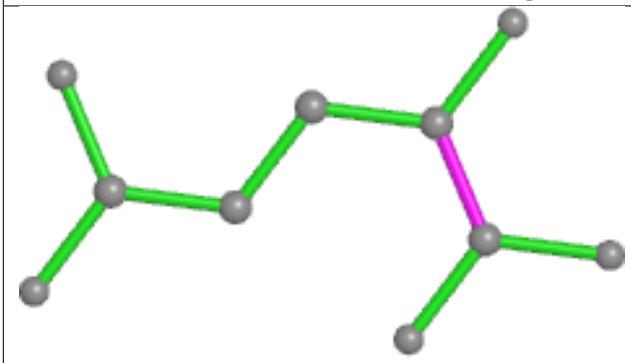
No monomer is involved in short contacts.

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.

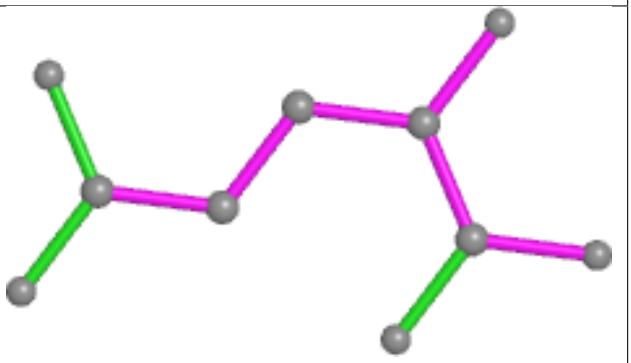
Ligand AKG A 402



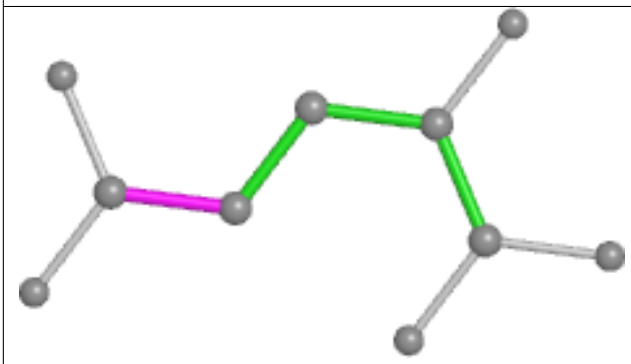
Ligand AKG B 402



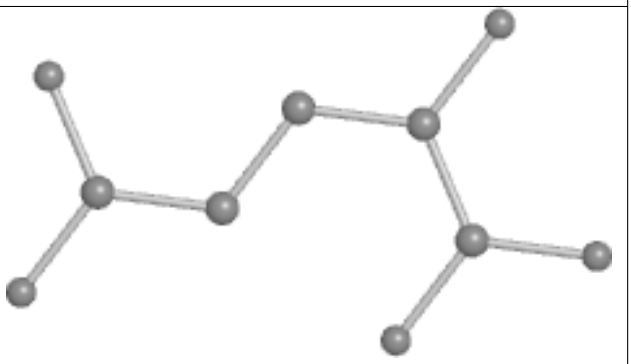
Bond lengths



Bond angles

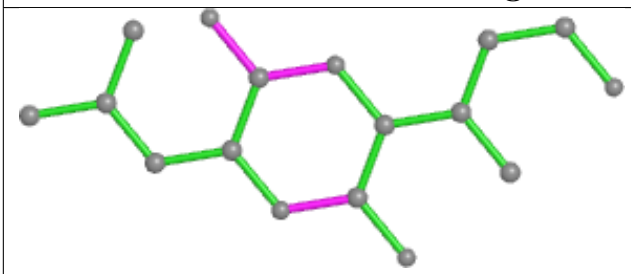


Torsions

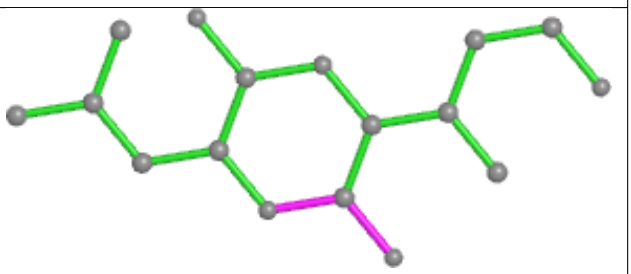


Rings

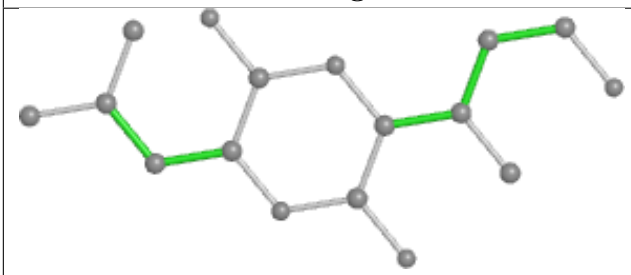
Ligand A1LVE A 404



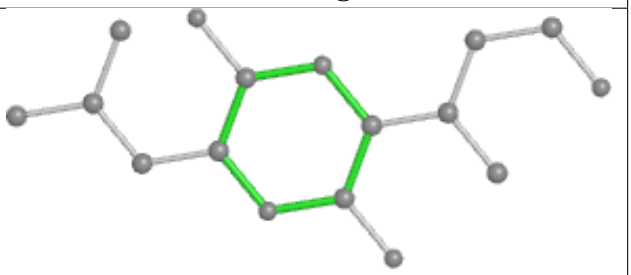
Bond lengths



Bond angles

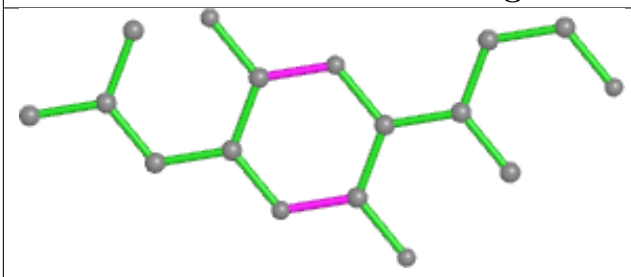


Torsions

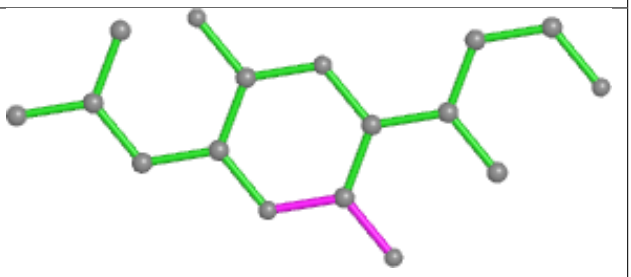


Rings

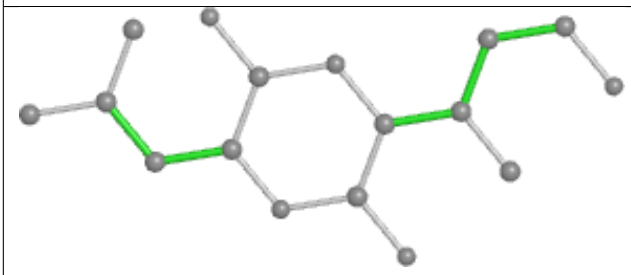
Ligand A1LVE D 404



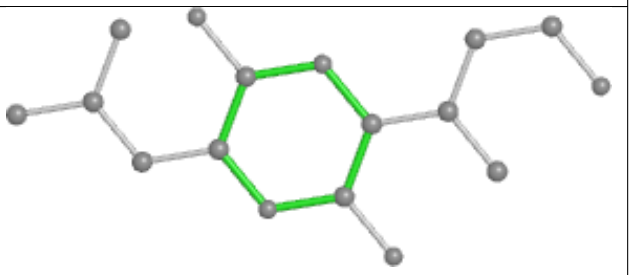
Bond lengths



Bond angles

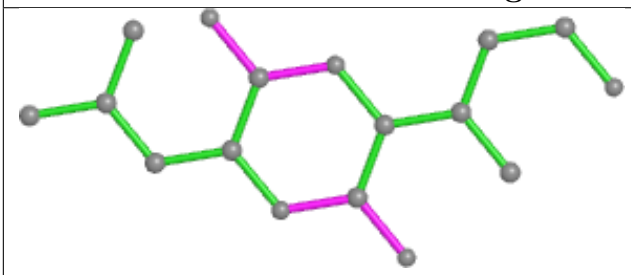


Torsions

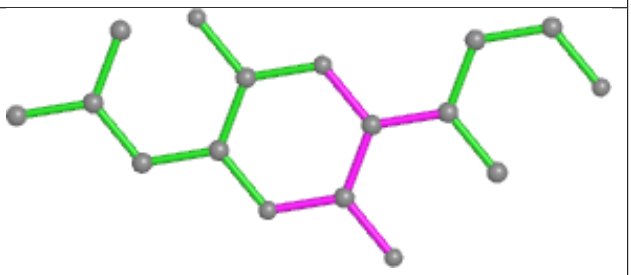


Rings

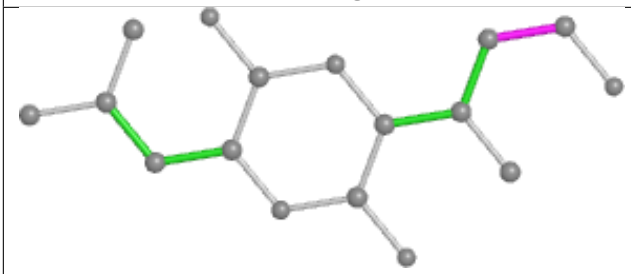
Ligand A1LVE C 403



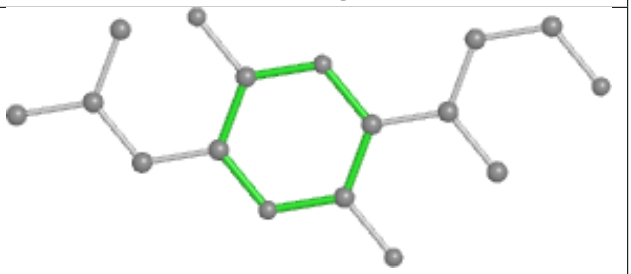
Bond lengths



Bond angles

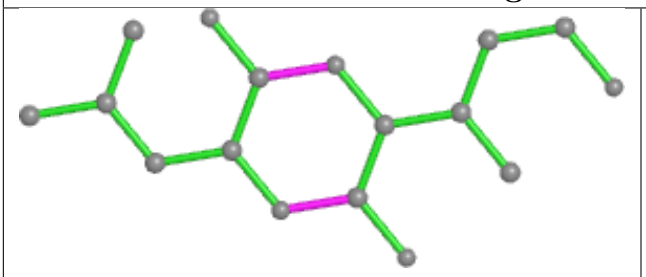


Torsions

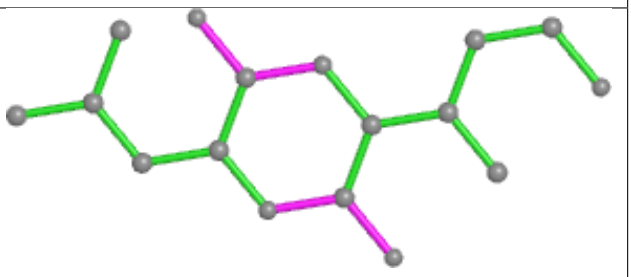


Rings

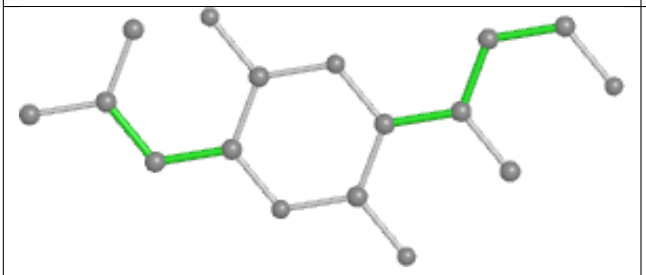
Ligand A1LVE B 403



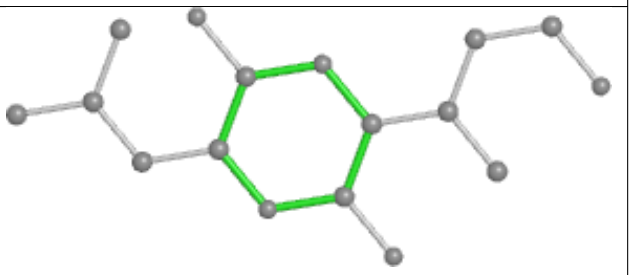
Bond lengths



Bond angles

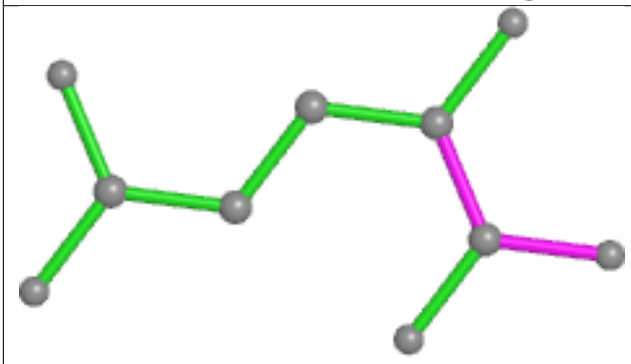


Torsions

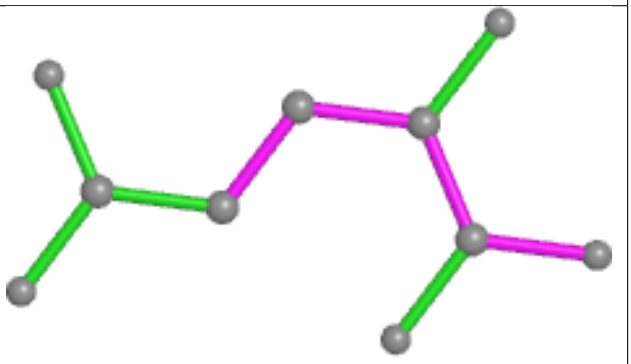


Rings

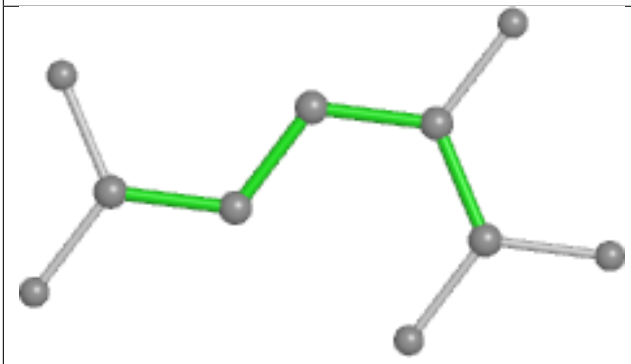
Ligand AKG C 402



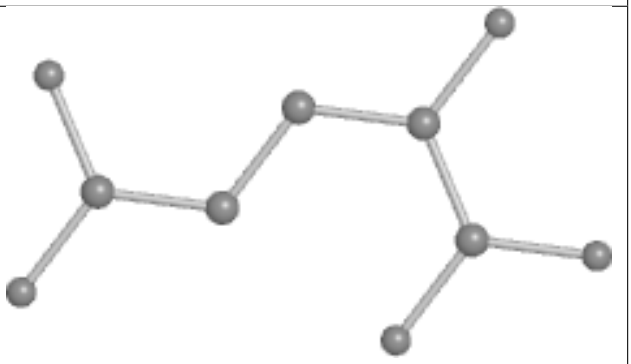
Bond lengths



Bond angles

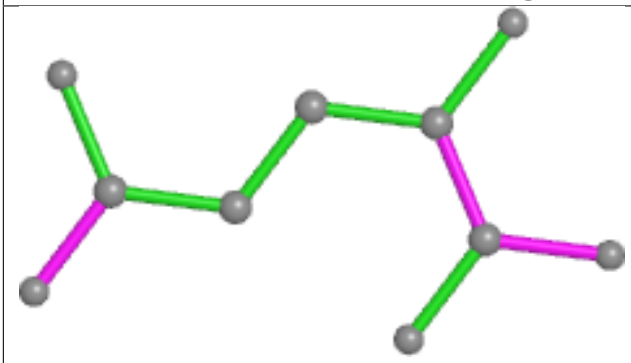


Torsions

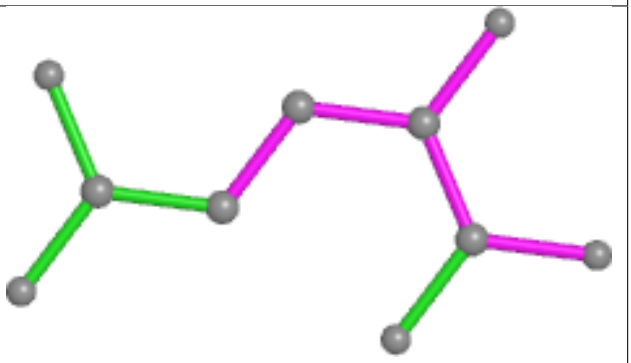


Rings

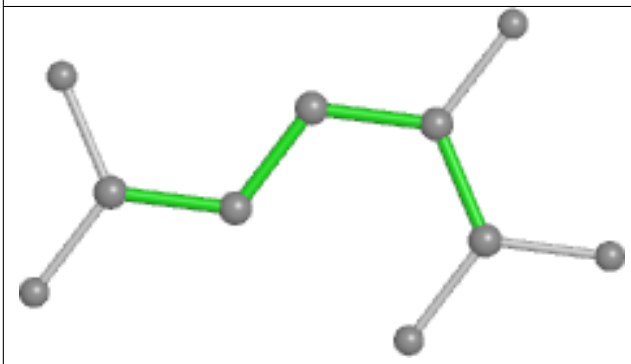
Ligand AKG D 402



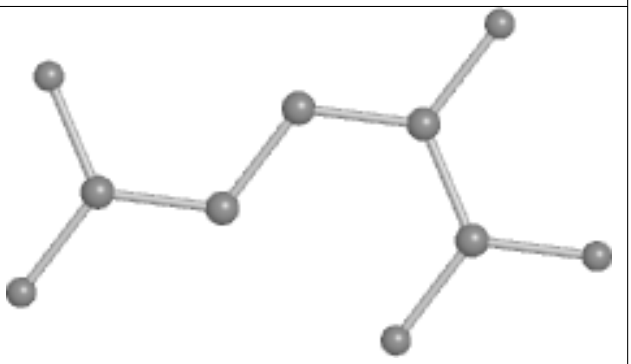
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	290/311 (93%)	-0.04	8 (2%) 55 57	10, 20, 38, 60	2 (0%)
1	B	289/311 (92%)	-0.09	7 (2%) 59 61	10, 19, 38, 60	3 (1%)
1	C	288/311 (92%)	0.51	30 (10%) 13 13	10, 24, 49, 66	3 (1%)
1	D	287/311 (92%)	0.53	20 (6%) 24 25	14, 27, 48, 76	4 (1%)
All	All	1154/1244 (92%)	0.23	65 (5%) 31 32	10, 22, 45, 76	12 (1%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	232	THR	4.9
1	D	234	PRO	4.2
1	D	235	ALA	4.0
1	D	232	THR	3.8
1	D	231	VAL	3.6
1	C	261	GLY	3.6
1	C	66	LEU	3.5
1	C	160	HIS	3.5
1	C	231	VAL	3.2
1	C	67	ARG	3.2
1	D	84[A]	TYR	3.1
1	B	291	THR	3.1
1	A	2	THR	2.9
1	C	69	TYR	2.9
1	C	188	GLY	2.9
1	A	215	ARG	2.8
1	B	61	PRO	2.8
1	C	236	ARG	2.8
1	C	259	GLU	2.8
1	D	66	LEU	2.7
1	D	236	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	6	MET	2.7
1	C	56	TYR	2.6
1	B	218	ARG	2.6
1	C	64	PRO	2.6
1	D	291	THR	2.6
1	C	62	GLY	2.5
1	A	16	GLY	2.5
1	C	291	THR	2.5
1	C	58	PRO	2.4
1	D	261	GLY	2.4
1	C	265	ALA	2.4
1	D	59	ALA	2.4
1	C	235	ALA	2.4
1	D	262	GLU	2.4
1	D	14	ALA	2.4
1	D	133	VAL	2.4
1	B	3	THR	2.4
1	C	59	ALA	2.3
1	C	218	ARG	2.3
1	C	233	GLU	2.3
1	B	62	GLY	2.3
1	D	233	GLU	2.3
1	D	264	VAL	2.3
1	D	60	HIS	2.3
1	A	264	VAL	2.2
1	D	266	VAL	2.2
1	C	75	ASN	2.2
1	B	7	THR	2.2
1	C	57	ARG	2.2
1	C	132	ALA	2.2
1	D	259	GLU	2.2
1	A	133	VAL	2.2
1	C	292	THR	2.1
1	C	54	GLN	2.1
1	A	132	ALA	2.1
1	B	17	GLU	2.1
1	D	83[A]	GLU	2.1
1	C	74	ARG	2.1
1	C	100	TYR	2.1
1	D	13	THR	2.1
1	C	70	ARG	2.1
1	A	14	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	17	GLU	2.0
1	C	258	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

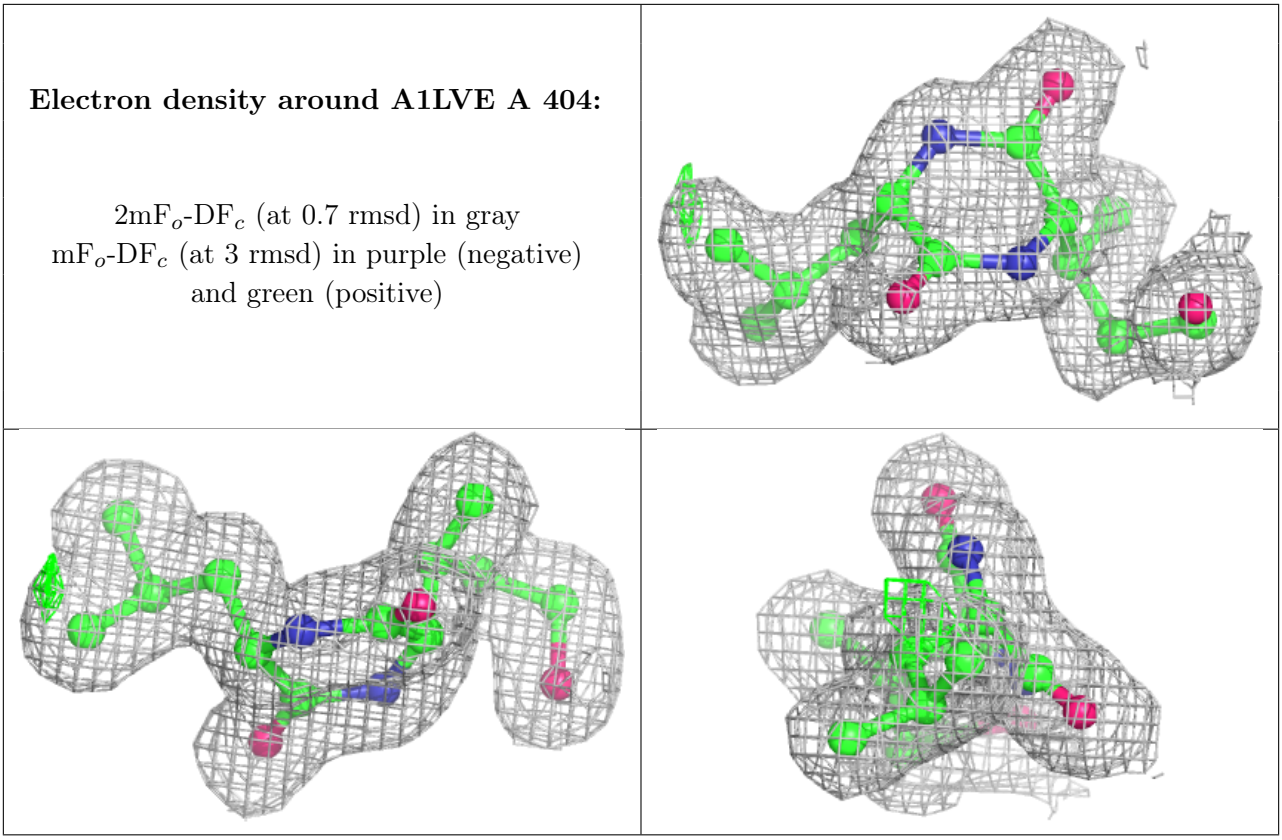
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	A1LVE	A	404	17/17	0.93	0.07	9,12,14,15	0
3	AKG	D	402	10/10	0.95	0.07	14,16,17,18	0
3	AKG	A	402	10/10	0.95	0.07	11,13,14,15	0
3	AKG	B	402	10/10	0.96	0.06	9,11,12,12	0
4	A1LVE	B	403	17/17	0.96	0.06	9,11,13,13	0
3	AKG	C	402	10/10	0.96	0.06	9,13,17,18	0
4	A1LVE	D	404	17/17	0.96	0.06	12,17,20,22	0
4	A1LVE	C	403	17/17	0.97	0.05	7,11,14,14	0
5	CL	D	403	1/1	0.98	0.14	38,38,38,38	0
2	FE2	D	401	1/1	0.99	0.03	16,16,16,16	0
2	FE2	C	401	1/1	0.99	0.04	12,12,12,12	0
2	FE2	A	401	1/1	1.00	0.06	11,11,11,11	0
2	FE2	B	401	1/1	1.00	0.03	9,9,9,9	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.

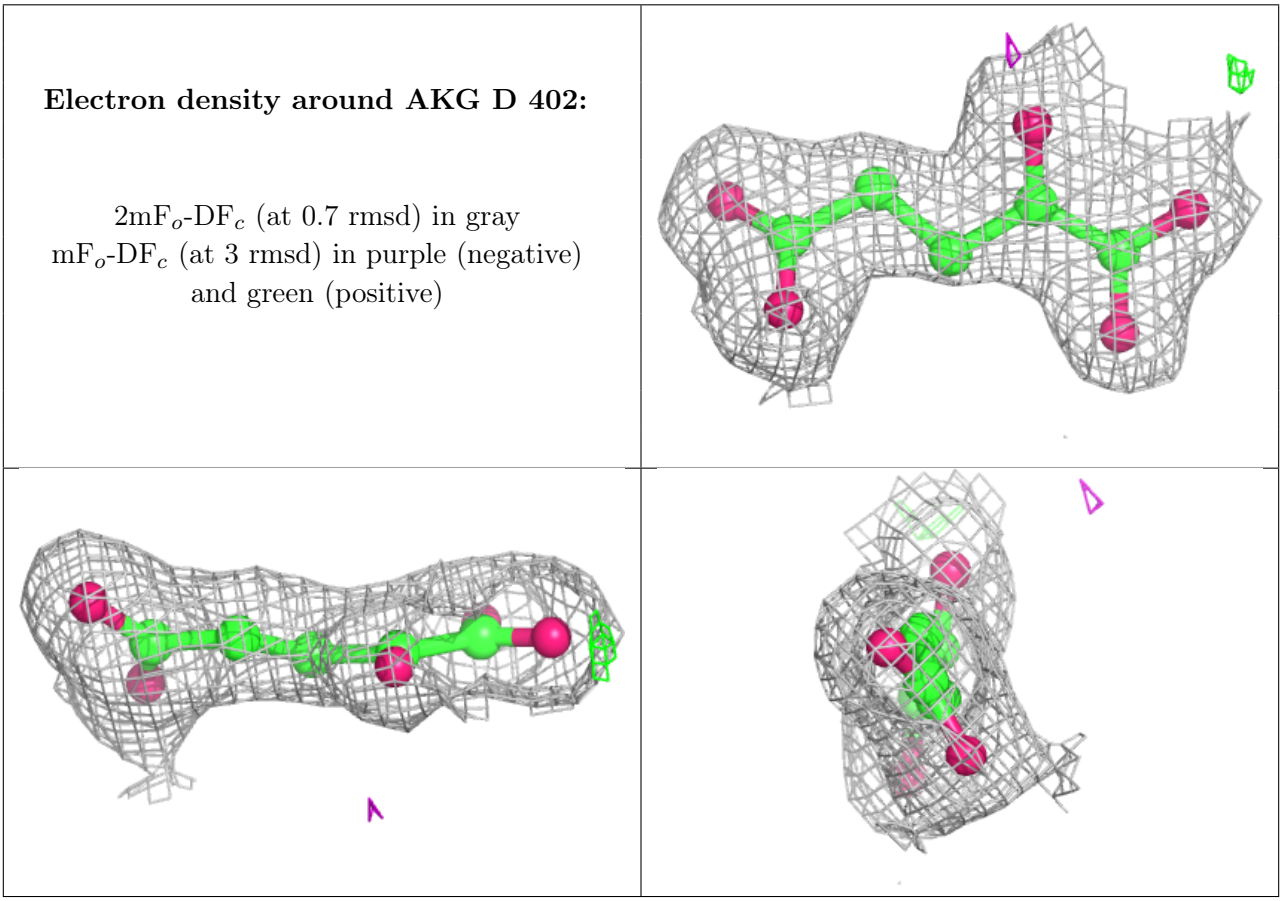
Electron density around A1LVE A 404:

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



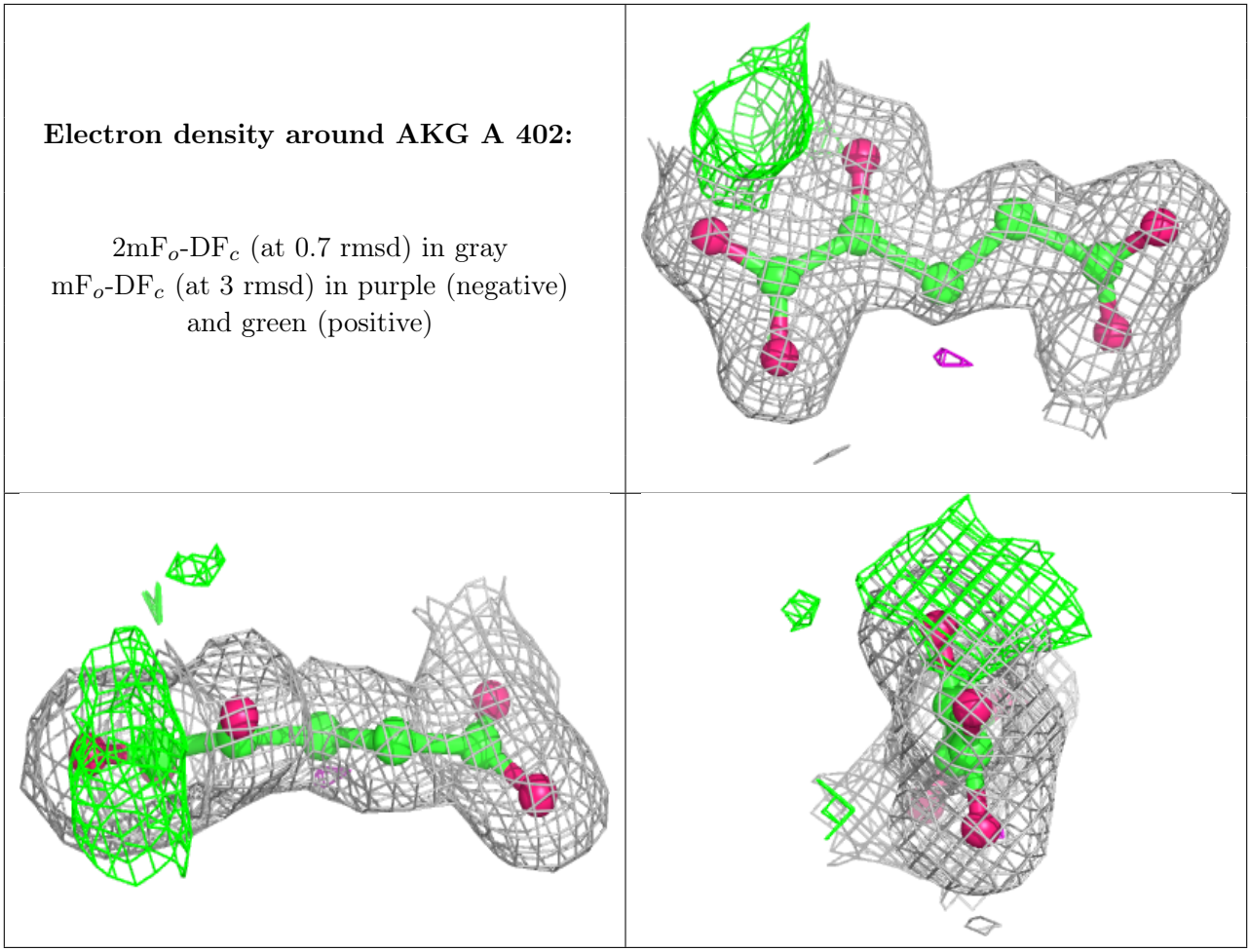
Electron density around AKG D 402:

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



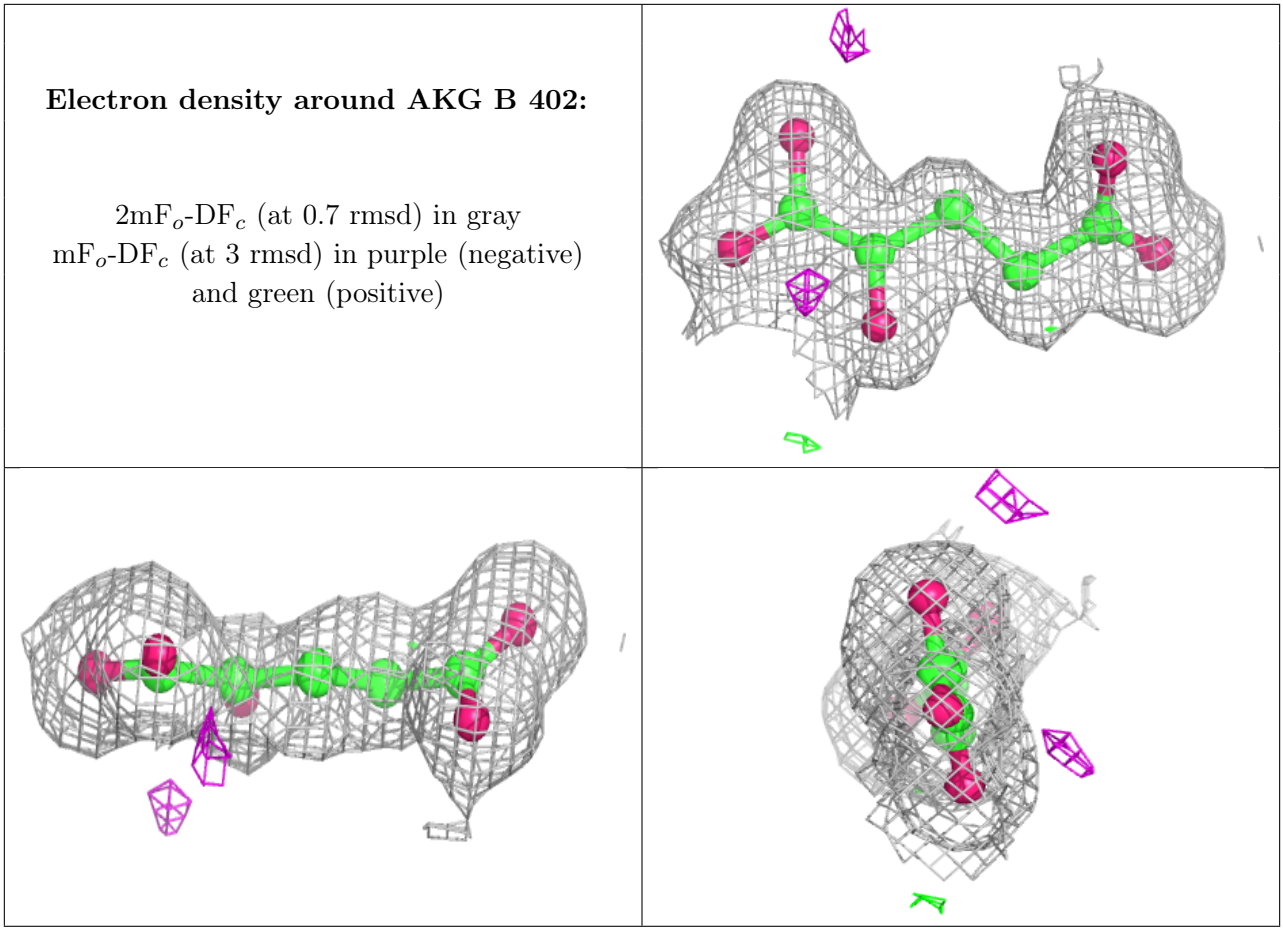
Electron density around AKG A 402:

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



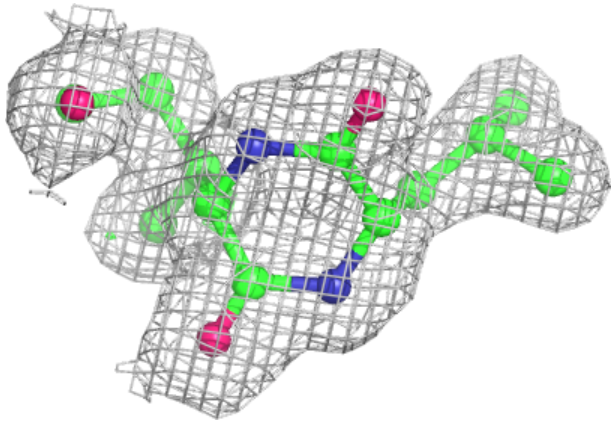
Electron density around AKG B 402:

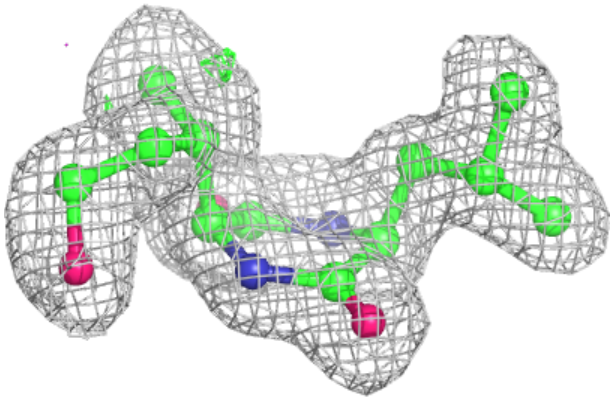
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

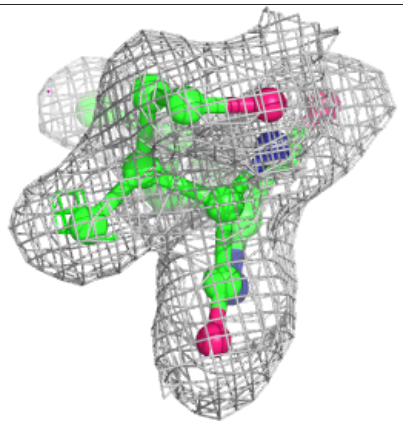


Electron density around A1LVE B 403:

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

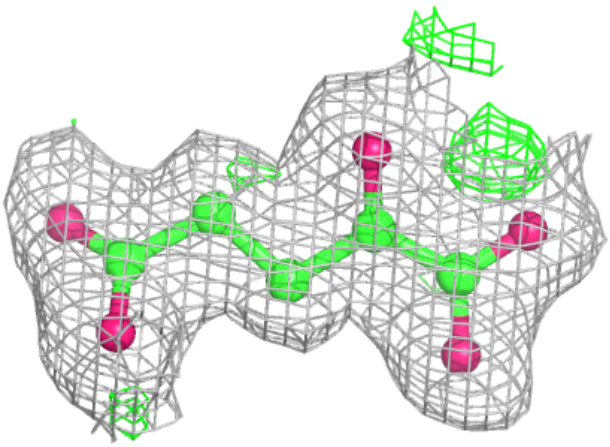


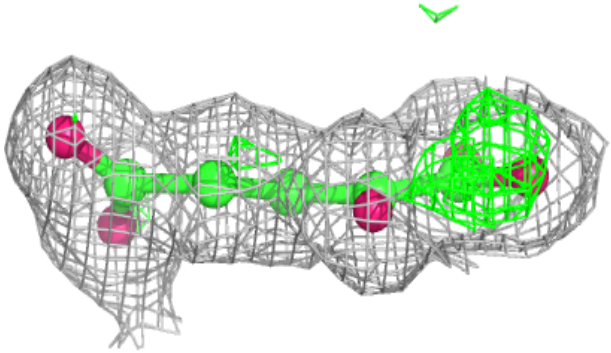


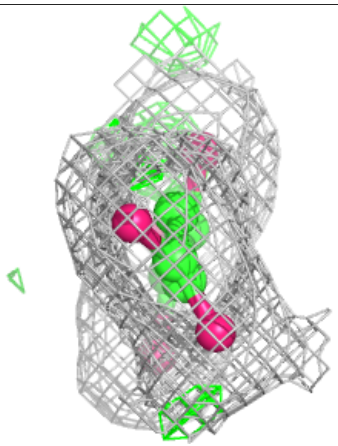


Electron density around AKG C 402:

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

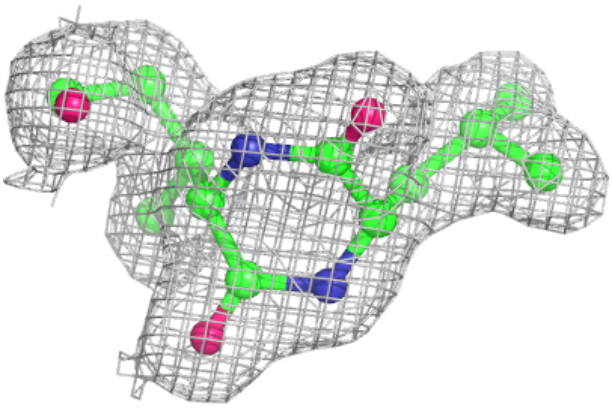


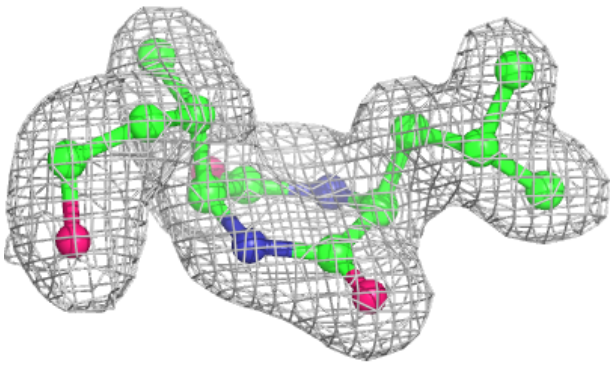




Electron density around A1LVE D 404:

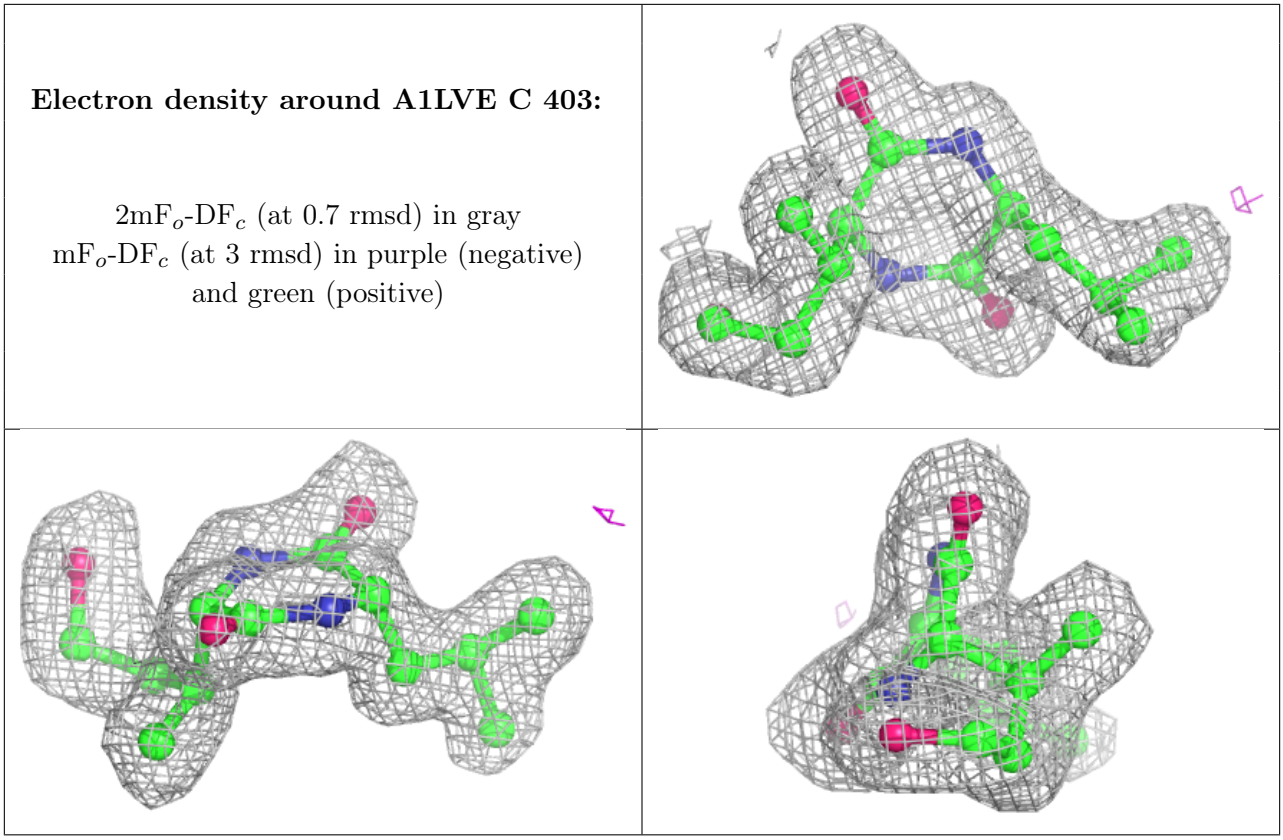
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around A1LVE C 403:

$2mF_o$-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.