Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:54 PM BST

PDB ID	:	6NX9
Title	:	ECAII(D90T,K162T) MUTANT IN COMPLEX WITH CITRATE AT PH 7
Authors	:	Lubkowski, J.; Wlodawer, A.
Deposited on	:	2019-02-08
Resolution	:	1.97 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 following versions of software and data (see references ⓘ) were used in the production of this report:

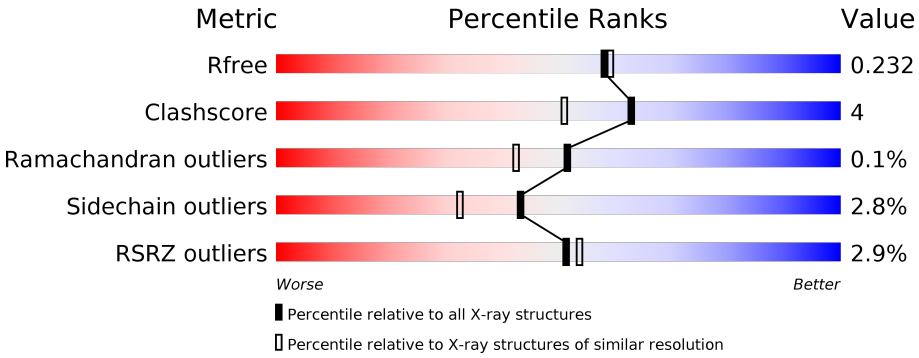
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 on 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	333	3% 82% 13% • •
1	B	333	5% 78% 14% • 7%
1	C	333	2% 81% 13% 6%
1	D	333	% 81% 12% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10529 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 L-asparaginase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	2	0
			2401	1502	411	480	8			
1	B	311	Total	C	N	O	S	0	0	0
			2331	1457	398	468	8			
1	C	313	Total	C	N	O	S	0	3	0
			2361	1475	404	474	8			
1	D	313	Total	C	N	O	S	0	1	0
			2348	1467	402	471	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P00805
A	-5	HIS	-	expression tag	UNP P00805
A	-4	HIS	-	expression tag	UNP P00805
A	-3	HIS	-	expression tag	UNP P00805
A	-2	HIS	-	expression tag	UNP P00805
A	-1	HIS	-	expression tag	UNP P00805
A	0	HIS	-	expression tag	UNP P00805
A	90	THR	ASP	conflict	UNP P00805
A	162	THR	LYS	engineered mutation	UNP P00805
B	-6	MET	-	initiating methionine	UNP P00805
B	-5	HIS	-	expression tag	UNP P00805
B	-4	HIS	-	expression tag	UNP P00805
B	-3	HIS	-	expression tag	UNP P00805
B	-2	HIS	-	expression tag	UNP P00805
B	-1	HIS	-	expression tag	UNP P00805
B	0	HIS	-	expression tag	UNP P00805
B	90	THR	ASP	conflict	UNP P00805
B	162	THR	LYS	engineered mutation	UNP P00805
C	-6	MET	-	initiating methionine	UNP P00805
C	-5	HIS	-	expression tag	UNP P00805
C	-4	HIS	-	expression tag	UNP P00805

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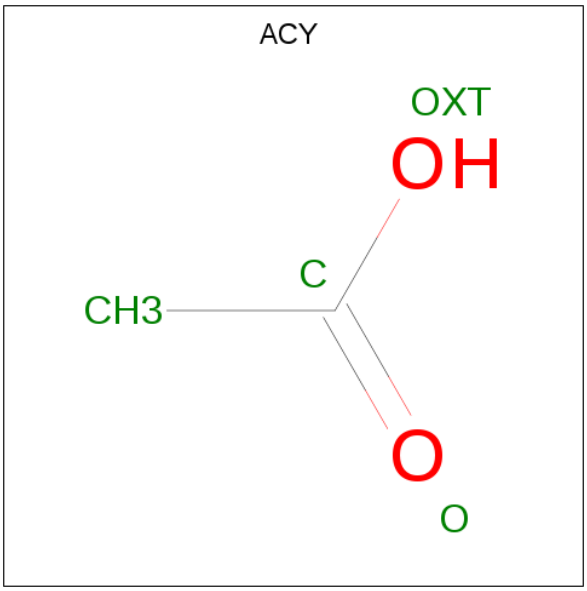
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP P00805
C	-2	HIS	-	expression tag	UNP P00805
C	-1	HIS	-	expression tag	UNP P00805
C	0	HIS	-	expression tag	UNP P00805
C	90	THR	ASP	conflict	UNP P00805
C	162	THR	LYS	engineered mutation	UNP P00805
D	-6	MET	-	initiating methionine	UNP P00805
D	-5	HIS	-	expression tag	UNP P00805
D	-4	HIS	-	expression tag	UNP P00805
D	-3	HIS	-	expression tag	UNP P00805
D	-2	HIS	-	expression tag	UNP P00805
D	-1	HIS	-	expression tag	UNP P00805
D	0	HIS	-	expression tag	UNP P00805
D	90	THR	ASP	conflict	UNP P00805
D	162	THR	LYS	engineered mutation	UNP P00805

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$) (labeled as "Ligand of Interest" by author).



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

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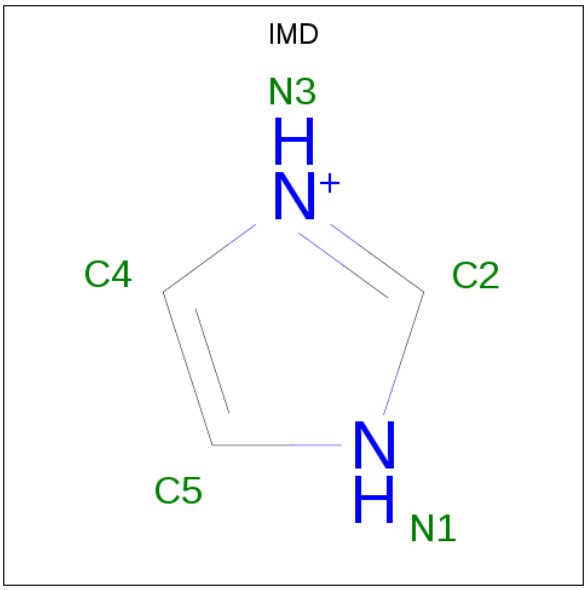
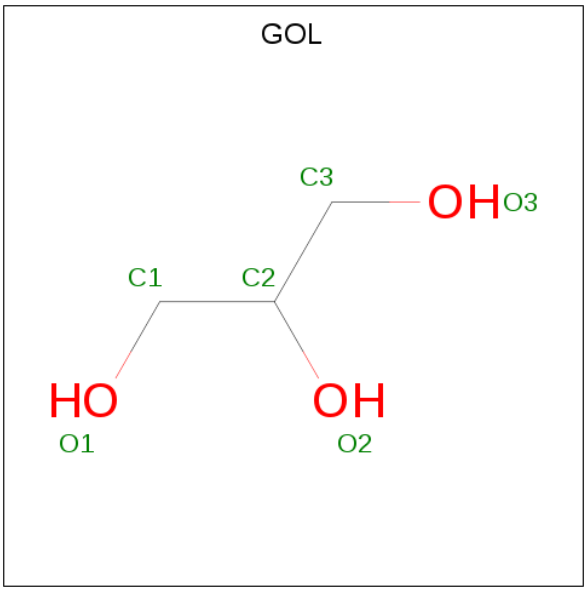
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by author).



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

- Molecule 5 is water.

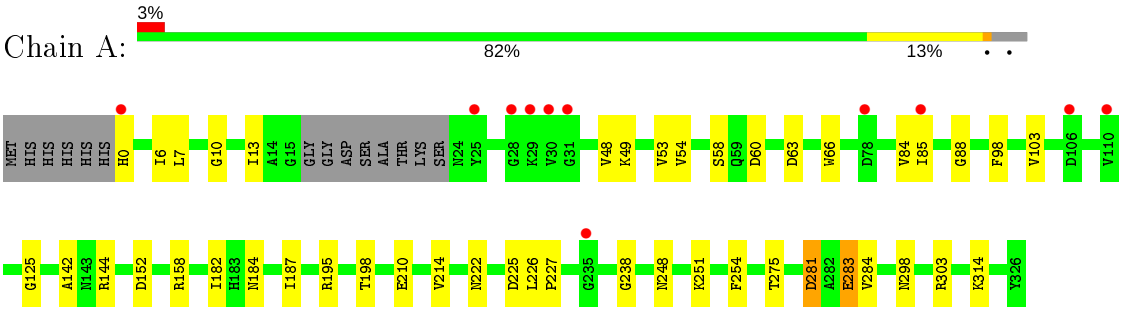
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	263	Total O 264 264	0	1
5	B	215	Total O 219 219	0	4
5	C	285	Total O 286 286	0	1
5	D	280	Total O 280 280	0	0

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.

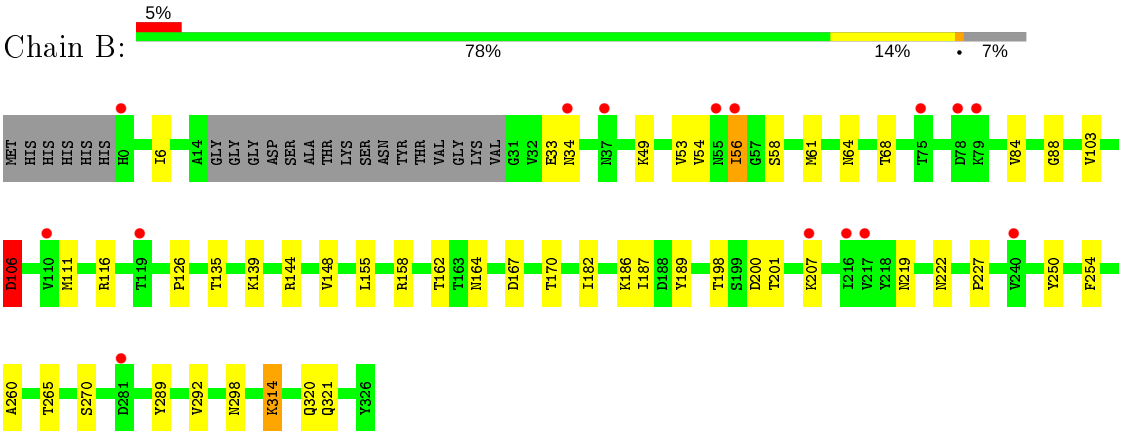
- Molecule 1: L-asparaginase 2

Chain A:



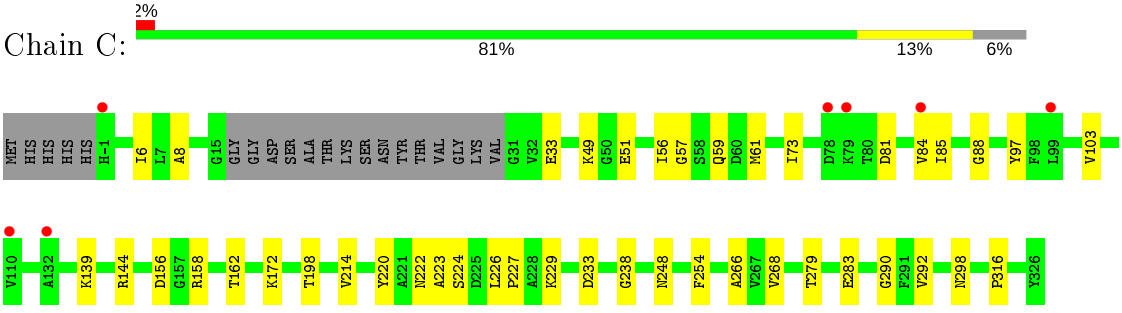
- Molecule 1: L-asparaginase 2

Chain B:



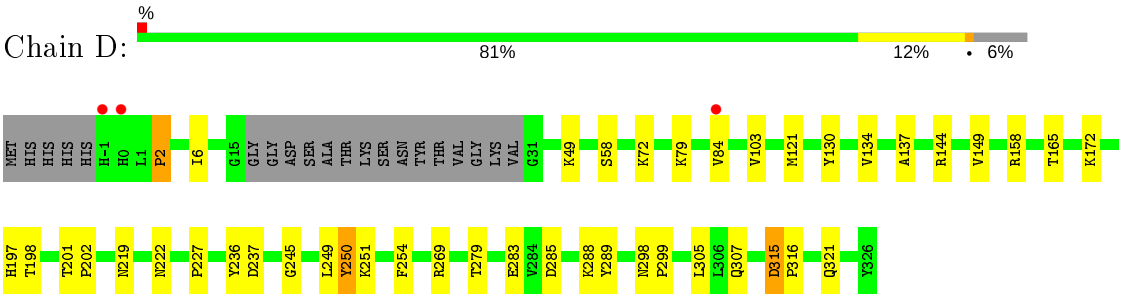
- Molecule 1: L-asparaginase 2

Chain C:



- Molecule 1: L-asparaginase 2

Chain D:


%
81%
12%
6%
MET HIS HIS HIS HIS H-1 H0 L1 P2 I6 G15 GLY GLY ASP SER ALA THR LYS SER ASN TYR THR VAL GLY LYS VAL G31 K49 S58 K72 K79 V84 V103 M121 Y130 V134 A137 R144 V149 R158 T165 K172
H197 T198 T201 P202 N219 N222 P227 Y236 D237 G245 L249 Y250 K251 F254 R269 T279 E283 V284 D285 K288 Y289 N298 P299 L305 L306 Q307 D315 P316 Q321 Y326

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.01Å 62.54Å 143.24Å 90.00° 118.19° 90.00°	Depositor
Resolution (Å)	26.55 – 1.97 26.54 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.3 (26.55-1.97) 96.3 (26.54-1.97)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.160 , 0.226 0.170 , 0.232	Depositor DCC
R_{free} test set	2654 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10529	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.88% 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: GOL, ACY, IMD

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	1.09	4/2445 (0.2%)	1.19	8/3332 (0.2%)
1	B	1.04	2/2367 (0.1%)	1.20	10/3226 (0.3%)
1	C	1.13	6/2407 (0.2%)	1.18	5/3281 (0.2%)
1	D	1.15	6/2388 (0.3%)	1.22	8/3254 (0.2%)
All	All	1.10	18/9607 (0.2%)	1.20	31/13093 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	GLU	CD-OE1	7.85	1.34	1.25
1	D	121	MET	C-O	7.24	1.37	1.23
1	D	245	GLY	C-O	6.70	1.34	1.23
1	C	8	ALA	C-O	6.69	1.36	1.23
1	C	88	GLY	C-O	6.54	1.34	1.23
1	C	266	ALA	C-O	5.85	1.34	1.23
1	D	58	SER	CA-CB	-5.79	1.44	1.52
1	D	249	LEU	C-O	5.77	1.34	1.23
1	A	210	GLU	CD-OE1	5.51	1.31	1.25
1	C	51	GLU	C-O	5.37	1.33	1.23
1	D	197	HIS	C-O	5.25	1.33	1.23
1	A	158	ARG	C-O	5.22	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	SER	C-O	5.22	1.33	1.23
1	A	10	GLY	C-O	5.12	1.31	1.23
1	B	135	THR	C-O	5.12	1.33	1.23
1	C	316	PRO	C-O	-5.12	1.13	1.23
1	C	57	GLY	C-O	5.10	1.31	1.23
1	D	305	LEU	C-O	5.04	1.32	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144	ARG	NE-CZ-NH2	-11.48	114.56	120.30
1	A	144	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	D	144	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	B	144	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	158	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	A	195	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	C	144	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	106	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	C	97	TYR	CB-CG-CD1	6.67	125.00	121.00
1	B	116	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	303	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	144	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	B	68	THR	CA-CB-OG1	-6.19	96.01	109.00
1	A	298	ASN	CB-CA-C	6.02	122.45	110.40
1	D	237	ASP	CB-CG-OD1	-6.02	112.88	118.30
1	B	158	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	289	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	D	2	PRO	N-CA-CB	5.67	110.11	103.30
1	D	289	TYR	CB-CG-CD1	-5.66	117.61	121.00
1	D	315	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	D	250	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	D	269	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	189	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	C	298	ASN	CB-CA-C	5.16	120.72	110.40
1	A	142	ALA	CB-CA-C	5.13	117.80	110.10
1	B	289	TYR	CB-CG-CD2	5.11	124.07	121.00
1	C	233	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	303	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	63	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	D	158	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	167	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ASP	Mainchain
1	D	307	GLN	Mainchain

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	2401	0	2395	18	0
1	B	2331	0	2323	19	0
1	C	2361	0	2351	22	0
1	D	2348	0	2338	24	0
2	A	4	0	3	1	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	5	0	5	0	0
4	C	12	0	16	2	0
4	D	6	0	8	3	0
5	A	264	0	0	4	0
5	B	219	0	0	4	0
5	C	286	0	0	9	0
5	D	280	0	0	11	0
All	All	10529	0	9448	81	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 4.

All (81) 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:B:321:GLN:NE2	5:B:501:HOH:O	1.91	1.01
1:C:279:THR:HG22	5:C:782:HOH:O	1.63	0.98
1:D:279:THR:HG22	5:D:879:HOH:O	1.83	0.79
1:D:279:THR:HG23	5:D:655:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:LYS:NZ	5:D:603:HOH:O	2.22	0.73
1:A:225:ASP:OD2	5:A:501:HOH:O	2.06	0.71
1:C:248[A]:ASN:OD1	1:C:283:GLU:HB3	1.90	0.71
1:D:202:PRO:HB3	4:D:501:GOL:H11	1.71	0.71
1:D:251:LYS:HE3	5:D:690:HOH:O	1.89	0.71
2:A:401:ACY:H1	5:A:574:HOH:O	1.96	0.65
1:C:59[B]:GLN:NE2	5:C:505:HOH:O	2.30	0.65
1:A:152:ASP:OD2	5:A:502:HOH:O	2.13	0.65
1:B:106:ASP:OD1	1:B:106:ASP:N	2.30	0.63
4:C:402:GOL:H11	5:D:694:HOH:O	2.00	0.61
1:C:49:LYS:HE3	5:C:678:HOH:O	2.00	0.60
1:B:219:ASN:HD22	1:B:250:TYR:H	1.50	0.59
1:B:260:ALA:HB1	1:B:265:THR:HB	1.85	0.58
1:C:290:GLY:O	5:C:502:HOH:O	2.18	0.57
1:A:103:VAL:O	1:A:198:THR:HA	2.05	0.56
1:A:182:ILE:HG12	1:A:187:ILE:HG12	1.88	0.55
1:B:34:ASN:HB3	5:B:670:HOH:O	2.05	0.55
1:D:298:ASN:HB2	1:D:299:PRO:CD	2.39	0.54
1:A:13:ILE:O	1:A:125:GLY:HA3	2.08	0.53
1:A:184:ASN:ND2	5:A:504:HOH:O	2.29	0.51
1:B:103:VAL:O	1:B:198:THR:HA	2.10	0.51
1:B:298:ASN:OD1	1:B:298:ASN:C	2.49	0.51
1:D:72:LYS:NZ	5:D:607:HOH:O	2.38	0.50
1:D:202:PRO:CA	4:D:501:GOL:H12	2.42	0.50
1:B:111:MET:HB2	1:B:148:VAL:HG22	1.94	0.49
1:B:182:ILE:HG12	1:B:187:ILE:HG12	1.94	0.49
1:C:81:ASP:OD1	5:C:503:HOH:O	2.20	0.49
1:B:162:THR:OG1	1:B:170:THR:OG1	2.23	0.49
1:D:219:ASN:HD22	1:D:250:TYR:H	1.58	0.49
1:A:281:ASP:HA	1:A:284:VAL:O	2.13	0.49
1:D:283:GLU:OE1	5:D:601:HOH:O	2.20	0.48
1:C:56:ILE:HD11	1:C:61:MET:HE1	1.96	0.48
1:B:56:ILE:HD12	1:B:61:MET:HE2	1.95	0.47
1:A:227:PRO:HB3	1:B:227:PRO:HB3	1.96	0.47
1:B:53:VAL:HG12	1:B:54:VAL:HG13	1.95	0.47
1:A:7:LEU:O	1:A:85:ILE:HA	2.15	0.47
1:C:268:VAL:HA	1:C:292:VAL:O	2.15	0.47
1:C:49:LYS:CE	5:C:678:HOH:O	2.60	0.47
1:C:6:ILE:HA	1:C:84:VAL:O	2.13	0.47
1:D:279:THR:CG2	5:D:655:HOH:O	2.51	0.47
1:D:103:VAL:O	1:D:198:THR:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ILE:HA	1:D:84:VAL:O	2.15	0.46
1:B:58:SER:HB3	1:B:88:GLY:HA3	1.97	0.46
1:C:227:PRO:HB3	1:D:227:PRO:HB3	1.96	0.46
1:A:66:TRP:HB3	1:A:98:PHE:CD2	2.50	0.46
1:B:314:LYS:HE2	5:B:507:HOH:O	2.14	0.46
1:C:49:LYS:HG3	5:C:678:HOH:O	2.16	0.46
1:A:214:VAL:HA	1:A:238:GLY:O	2.16	0.46
1:C:139:LYS:HG3	5:C:617:HOH:O	2.16	0.45
1:C:254:PHE:CD1	1:C:254:PHE:C	2.90	0.45
1:A:58:SER:HB3	1:A:88:GLY:HA3	1.98	0.45
1:D:202:PRO:HA	4:D:501:GOL:H12	1.98	0.45
1:A:53:VAL:HG12	1:A:54:VAL:HG13	1.99	0.45
1:D:2:PRO:HG2	1:D:137:ALA:HB1	1.98	0.45
1:C:214:VAL:HA	1:C:238:GLY:O	2.18	0.44
1:C:162:THR:O	1:C:162:THR:HG23	2.17	0.44
1:B:6:ILE:HA	1:B:84:VAL:O	2.18	0.44
1:C:226:LEU:HB2	1:C:227:PRO:HD3	2.00	0.44
1:B:314:LYS:CE	5:B:507:HOH:O	2.64	0.44
1:C:229:LYS:HE2	5:C:569:HOH:O	2.18	0.44
1:C:103:VAL:O	1:C:198:THR:HA	2.18	0.43
1:B:292:VAL:HG13	1:B:320:GLN:HA	2.00	0.43
1:C:73:ILE:HD11	1:C:85:ILE:HD11	1.99	0.43
1:A:226:LEU:N	1:A:227:PRO:CD	2.81	0.43
1:A:6:ILE:HA	1:A:84:VAL:O	2.19	0.43
1:D:149:VAL:HG12	5:D:633:HOH:O	2.19	0.43
1:D:172:LYS:HD3	5:D:699:HOH:O	2.19	0.43
1:A:275:THR:O	1:B:164:ASN:HA	2.18	0.43
1:A:6:ILE:HD12	1:A:48:VAL:CG1	2.48	0.42
4:C:402:GOL:H32	1:D:165:THR:O	2.19	0.42
1:C:220:TYR:CE2	1:C:223:ALA:HA	2.54	0.41
1:D:285:ASP:CG	1:D:288:LYS:HB2	2.40	0.41
1:D:321:GLN:HG3	5:D:867:HOH:O	2.20	0.41
1:C:224:SER:HB2	1:D:236:TYR:OH	2.20	0.41
1:A:248[B]:ASN:OD1	1:A:283:GLU:HB3	2.21	0.40
1:D:130:TYR:O	1:D:134:VAL:HG23	2.20	0.40
1:D:315:ASP:HA	1:D:316:PRO:HD3	1.97	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	317/333 (95%)	310 (98%)	6 (2%)	1 (0%)	41 29
1	B	307/333 (92%)	300 (98%)	7 (2%)	0	100 100
1	C	312/333 (94%)	308 (99%)	4 (1%)	0	100 100
1	D	310/333 (93%)	302 (97%)	8 (3%)	0	100 100
All	All	1246/1332 (94%)	1220 (98%)	25 (2%)	1 (0%)	51 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ASP

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	264/273 (97%)	258 (98%)	6 (2%)	50 44
1	B	256/273 (94%)	241 (94%)	15 (6%)	19 8
1	C	260/273 (95%)	256 (98%)	4 (2%)	65 59
1	D	258/273 (94%)	254 (98%)	4 (2%)	62 56
All	All	1038/1092 (95%)	1009 (97%)	29 (3%)	43 32

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	49	LYS
1	A	222	ASN
1	A	251	LYS
1	A	254	PHE
1	A	314	LYS
1	B	33	GLU
1	B	49	LYS
1	B	56	ILE
1	B	64	ASN
1	B	106	ASP
1	B	126	PRO
1	B	139	LYS
1	B	155	LEU
1	B	186	LYS
1	B	200	ASP
1	B	201	THR
1	B	207	LYS
1	B	222	ASN
1	B	254	PHE
1	B	314	LYS
1	C	33	GLU
1	C	156	ASP
1	C	172	LYS
1	C	222	ASN
1	D	49	LYS
1	D	201	THR
1	D	222	ASN
1	D	254	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	280	GLN
1	A	317	GLN
1	B	47	ASN
1	B	219	ASN
1	B	280	GLN
1	B	324	ASN
1	C	34	ASN
1	D	183	HIS
1	D	219	ASN

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Mol	Chain	Res	Type
1	D	312	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	C	402	-	5,5,5	0.66	0	5,5,5	1.65	1 (20%)
3	IMD	A	402	-	3,5,5	0.26	0	4,5,5	0.40	0
2	ACY	B	401	-	1,3,3	6.01	1 (100%)	0,3,3	0.00	-
2	ACY	A	401	-	1,3,3	5.06	1 (100%)	0,3,3	0.00	-
2	ACY	C	401	-	1,3,3	6.79	1 (100%)	0,3,3	0.00	-
4	GOL	D	501	-	5,5,5	0.30	0	5,5,5	0.98	0
2	ACY	D	502	-	1,3,3	4.84	1 (100%)	0,3,3	0.00	-
4	GOL	C	403	-	5,5,5	0.23	0	5,5,5	0.88	0

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
4	GOL	C	403	-	-	0/4/4/4	-
4	GOL	C	402	-	-	3/4/4/4	-
4	GOL	D	501	-	-	4/4/4/4	-
3	IMD	A	402	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ACY	CH3-C	6.79	1.57	1.48
2	B	401	ACY	CH3-C	6.01	1.56	1.48
2	A	401	ACY	CH3-C	5.06	1.55	1.48
2	D	502	ACY	CH3-C	4.84	1.54	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	402	GOL	O1-C1-C2	2.61	122.71	110.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	402	GOL	C1-C2-C3-O3
4	D	501	GOL	O1-C1-C2-O2
4	D	501	GOL	O1-C1-C2-C3
4	D	501	GOL	C1-C2-C3-O3
4	C	402	GOL	O1-C1-C2-C3
4	D	501	GOL	O2-C2-C3-O3
4	C	402	GOL	O1-C1-C2-O2

There are no ring outliers.

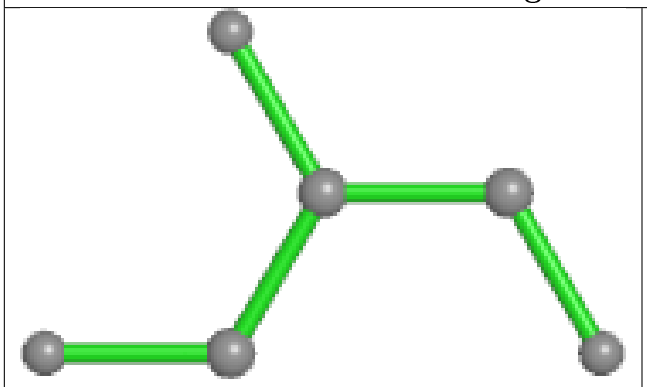
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	GOL	2	0
2	A	401	ACY	1	0
4	D	501	GOL	3	0

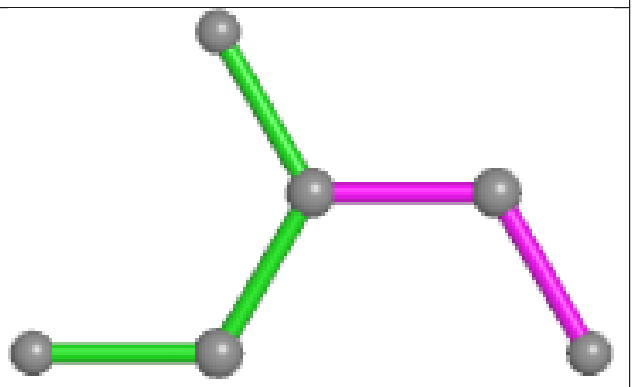
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

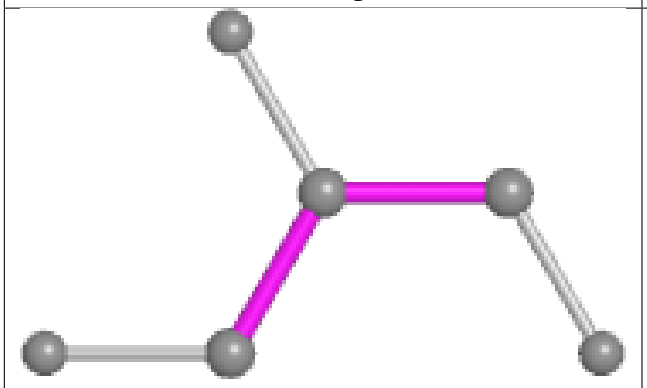
Ligand GOL C 402



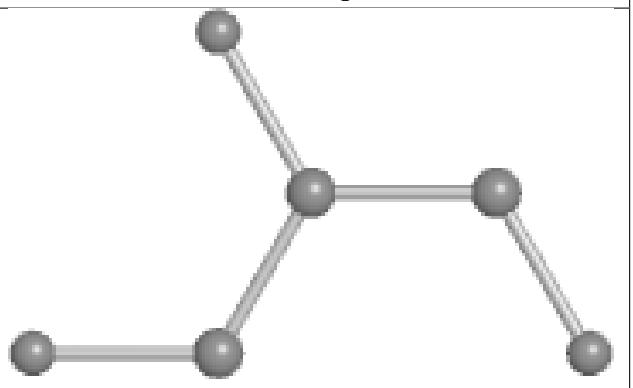
Bond lengths



Bond angles

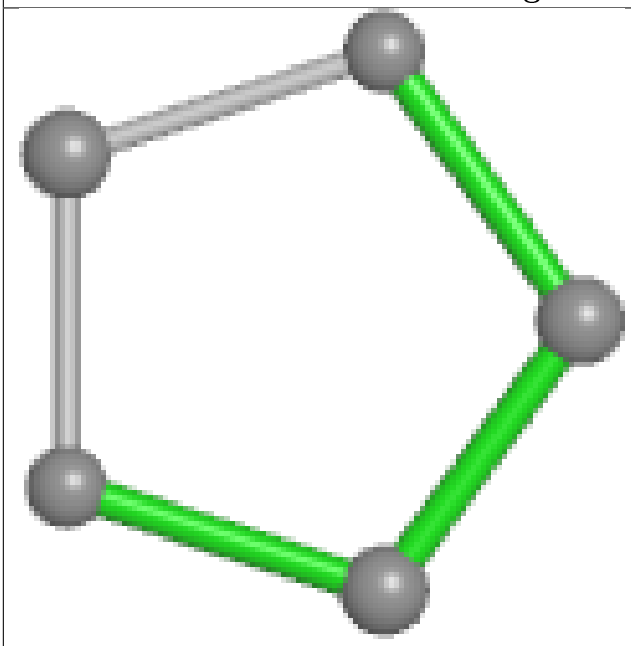


Torsions

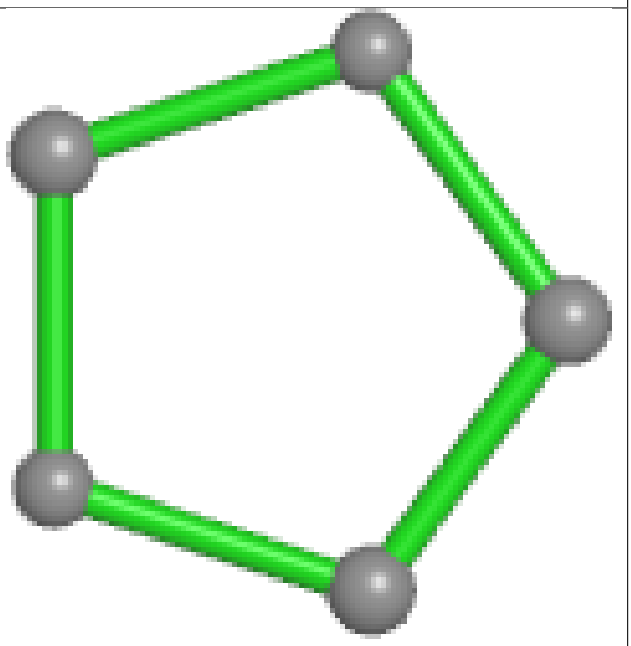


Rings

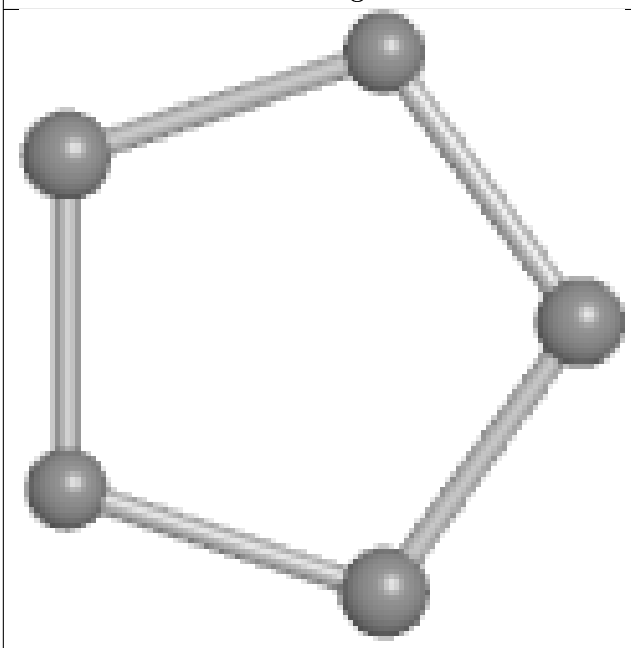
Ligand IMD A 402



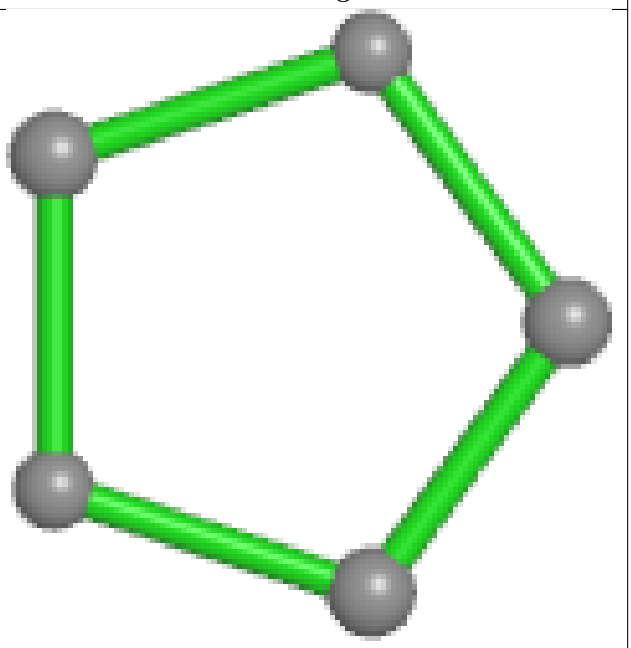
Bond lengths



Bond angles

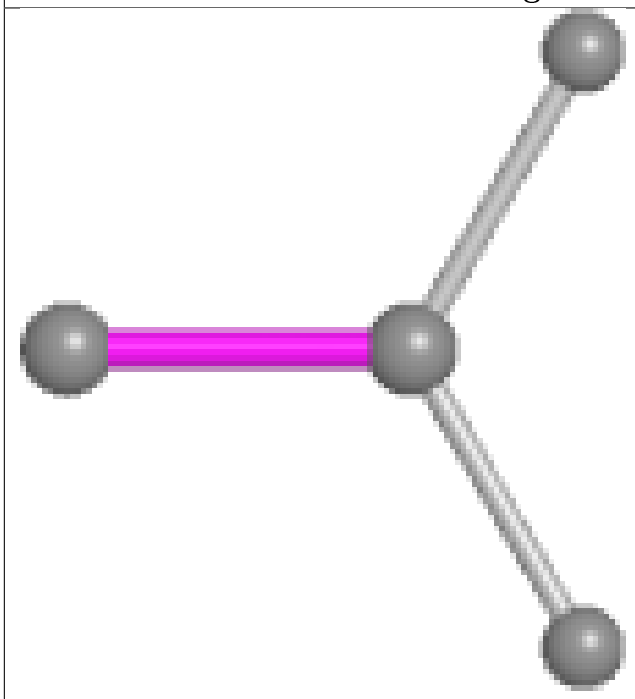


Torsions

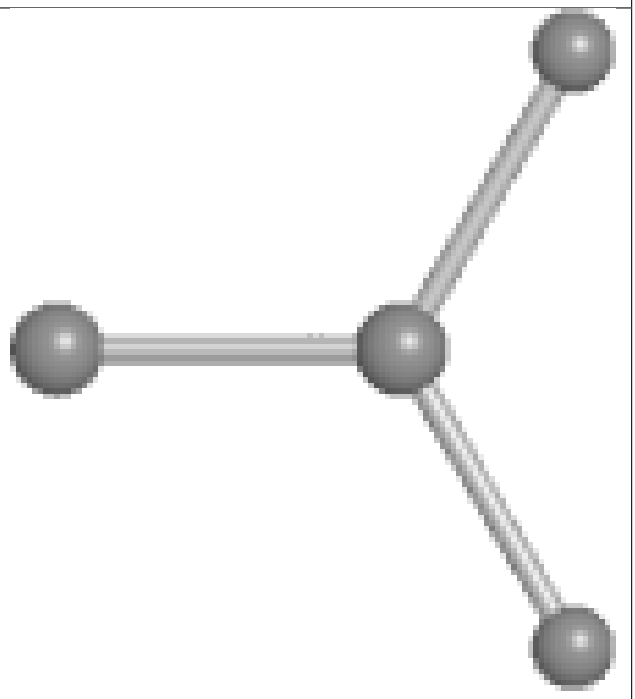


Rings

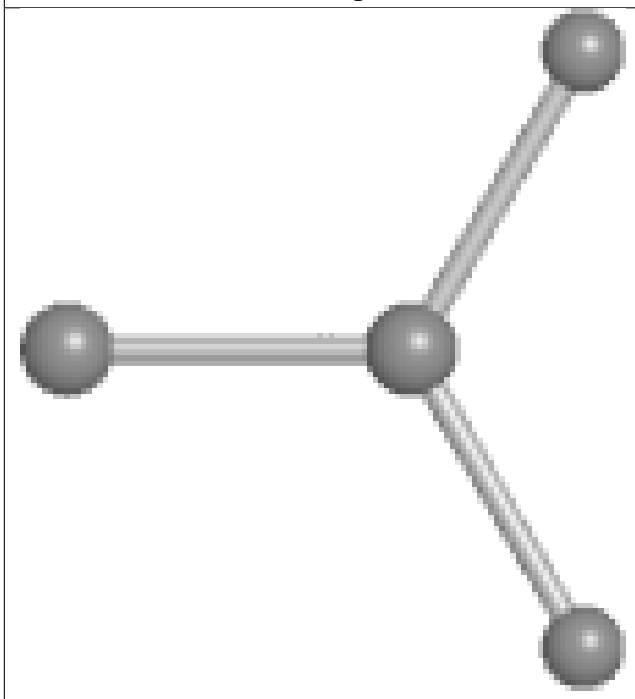
Ligand ACY B 401



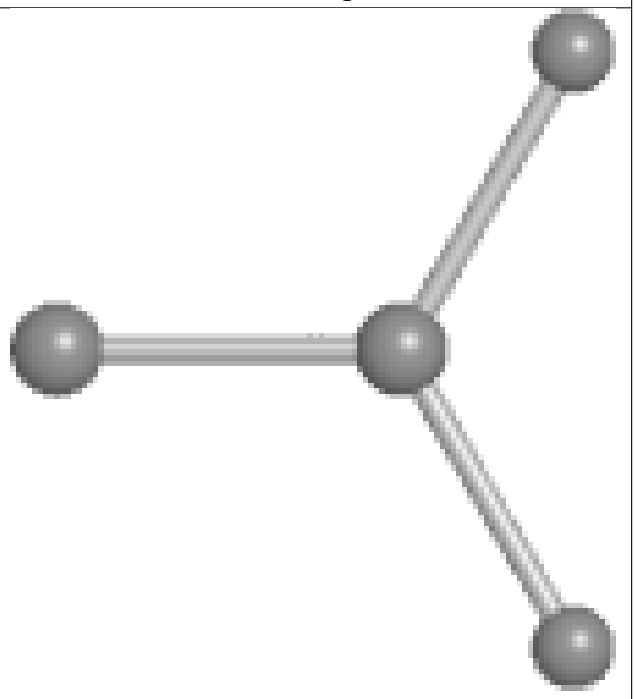
Bond lengths



Bond angles

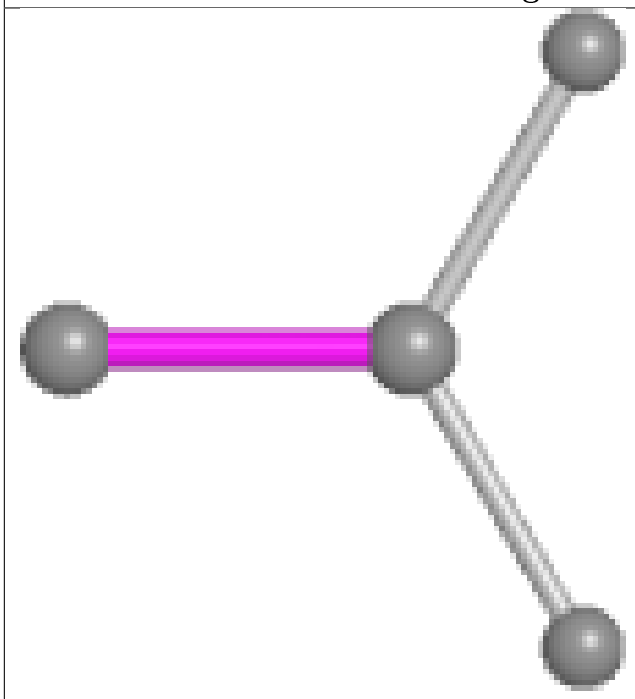


Torsions

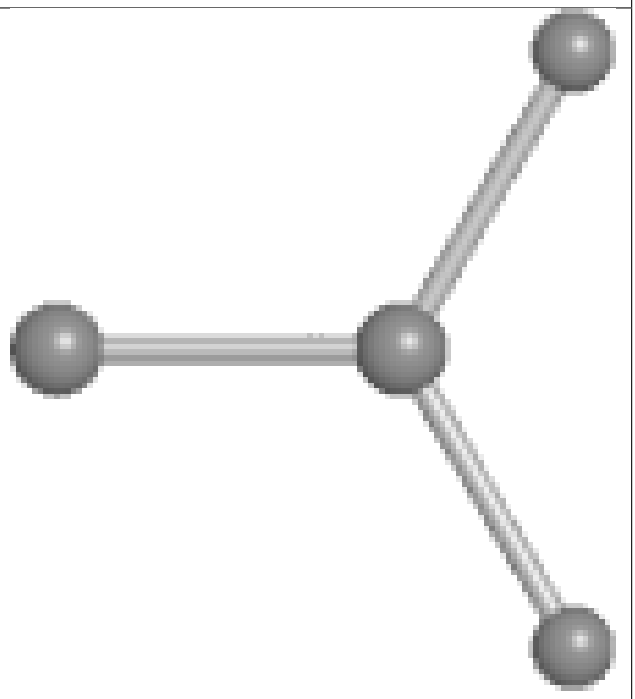


Rings

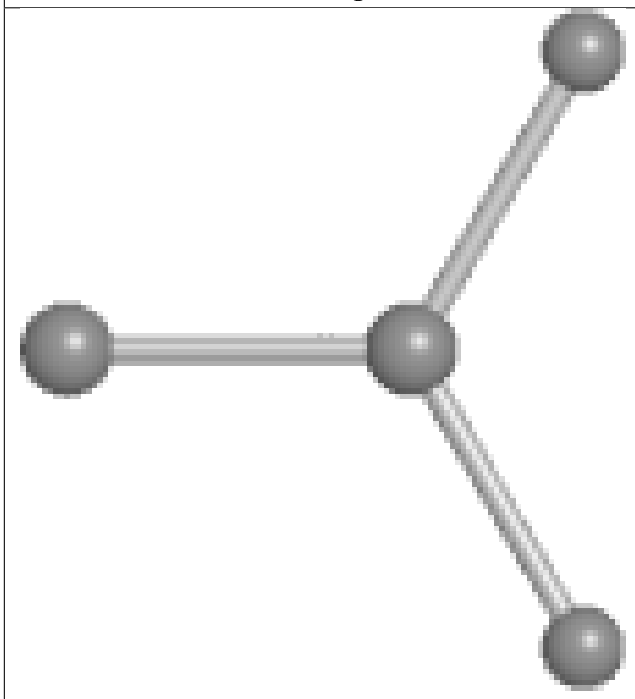
Ligand ACY A 401



Bond lengths



Bond angles



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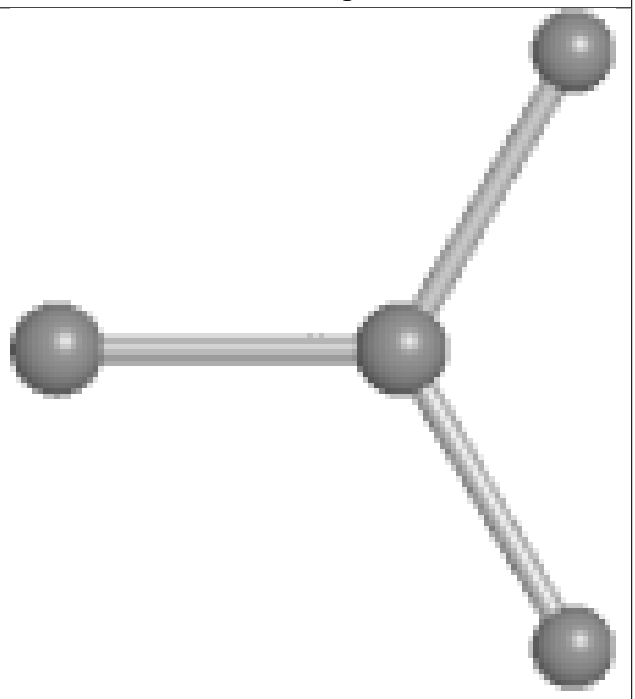
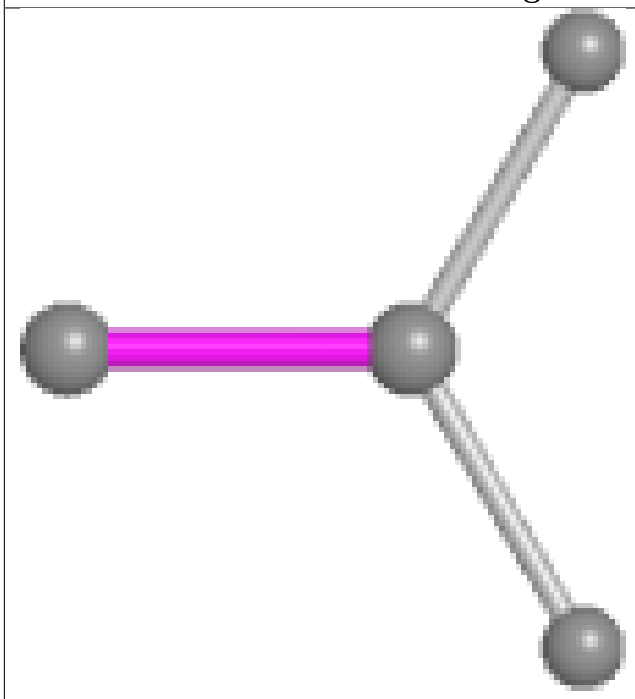
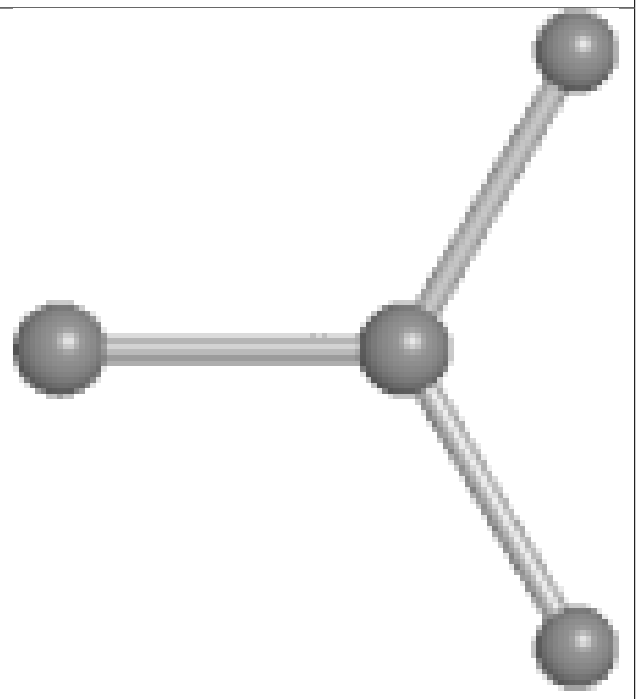


Rings

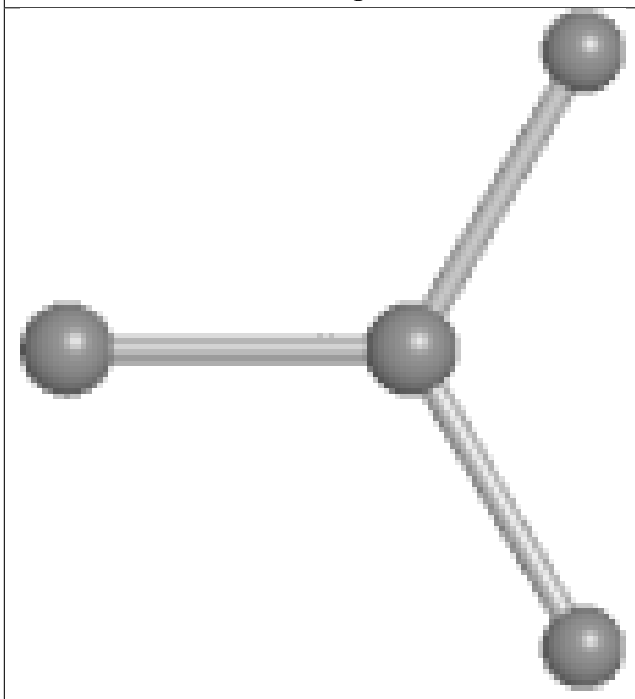
Ligand ACY C 401



Bond lengths



Bond angles



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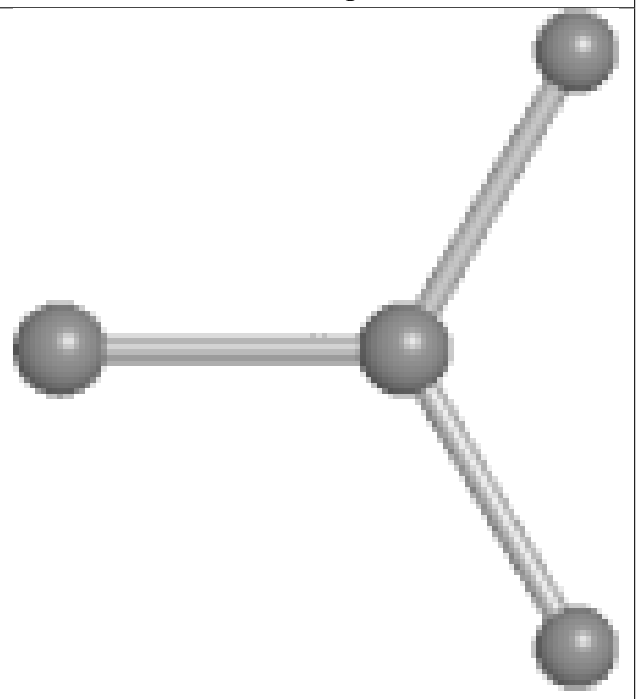
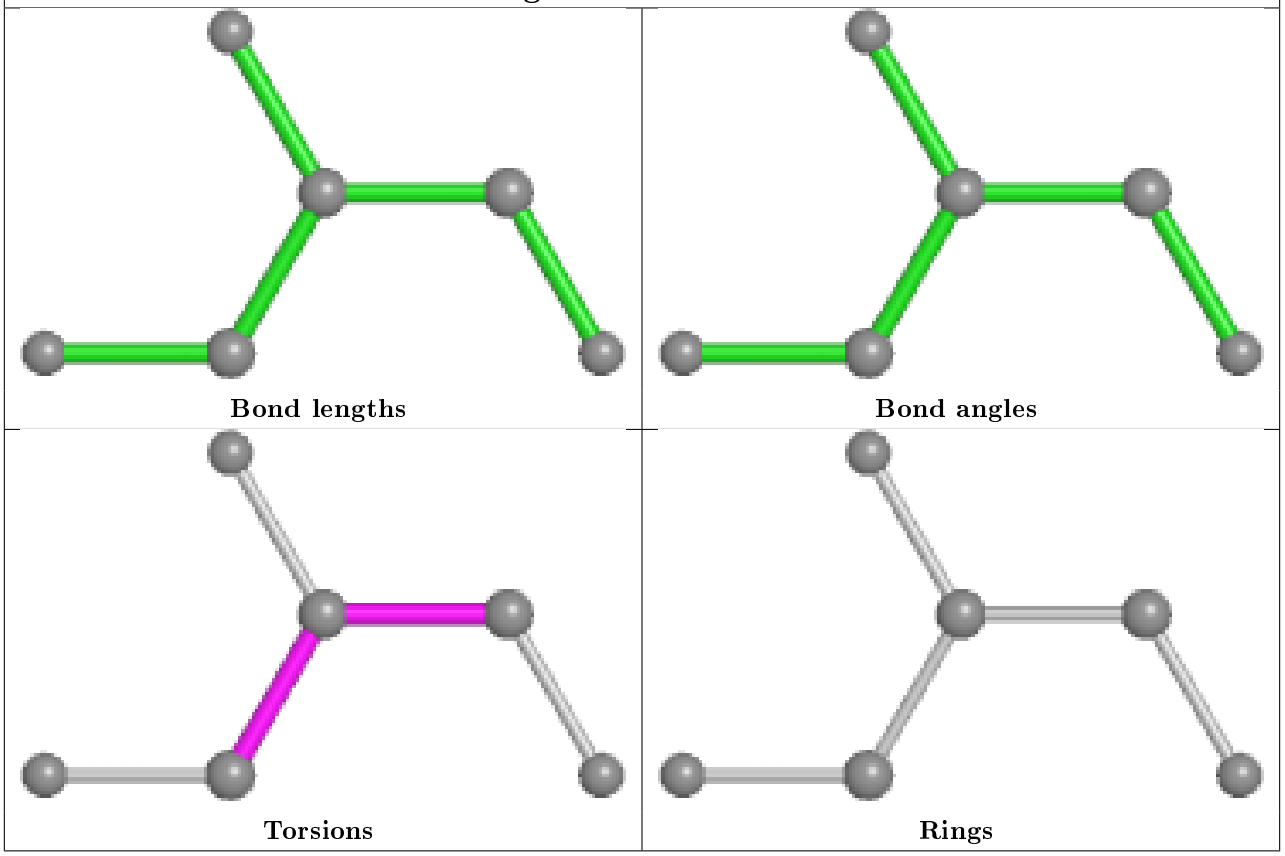
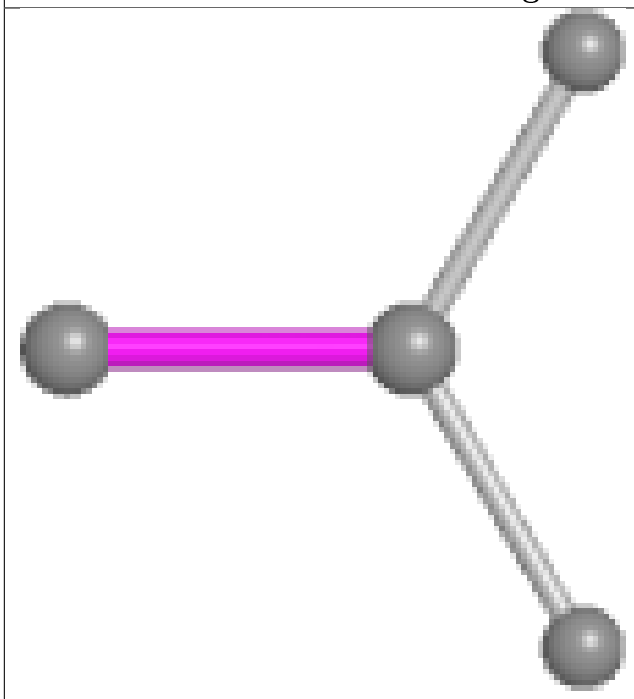


Rings

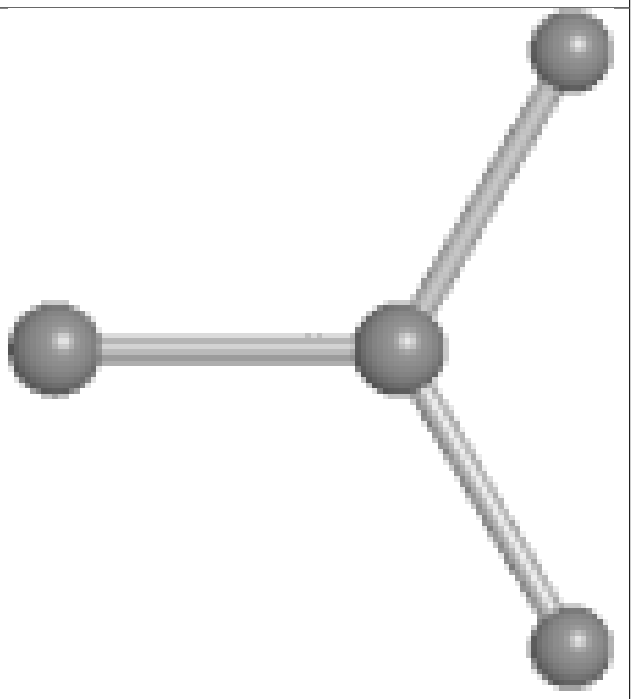
Ligand GOL D 501



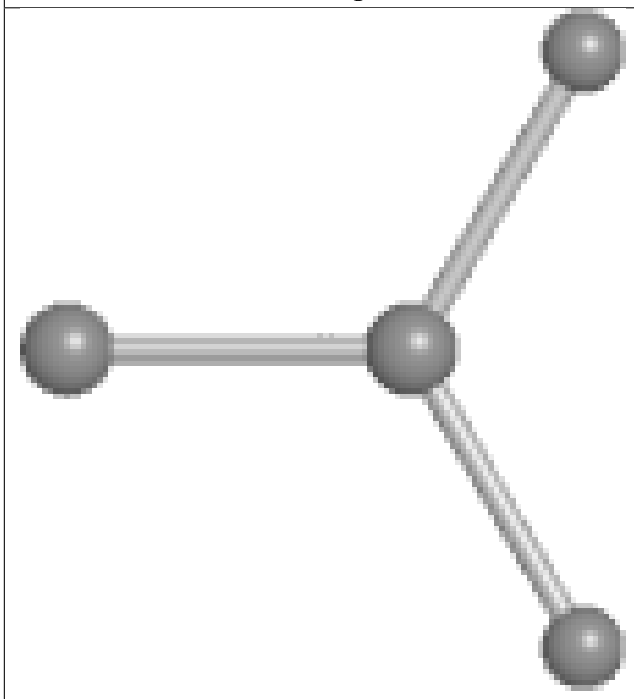
Ligand ACY D 502



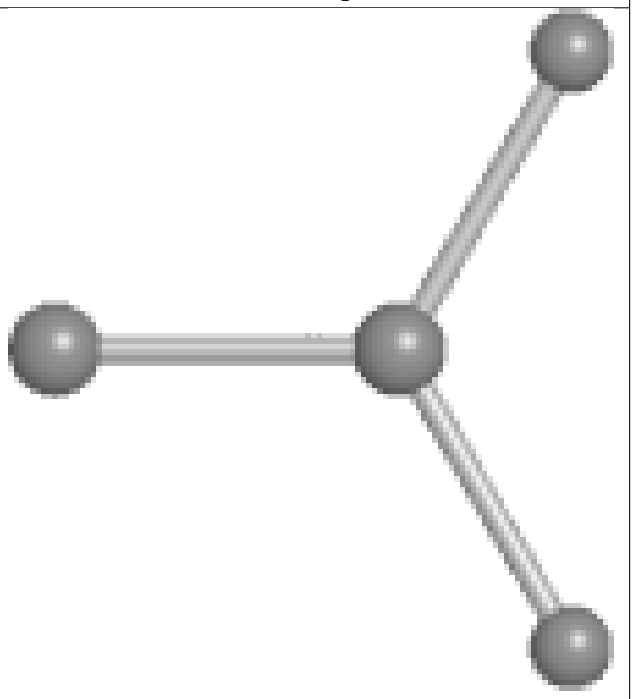
Bond lengths



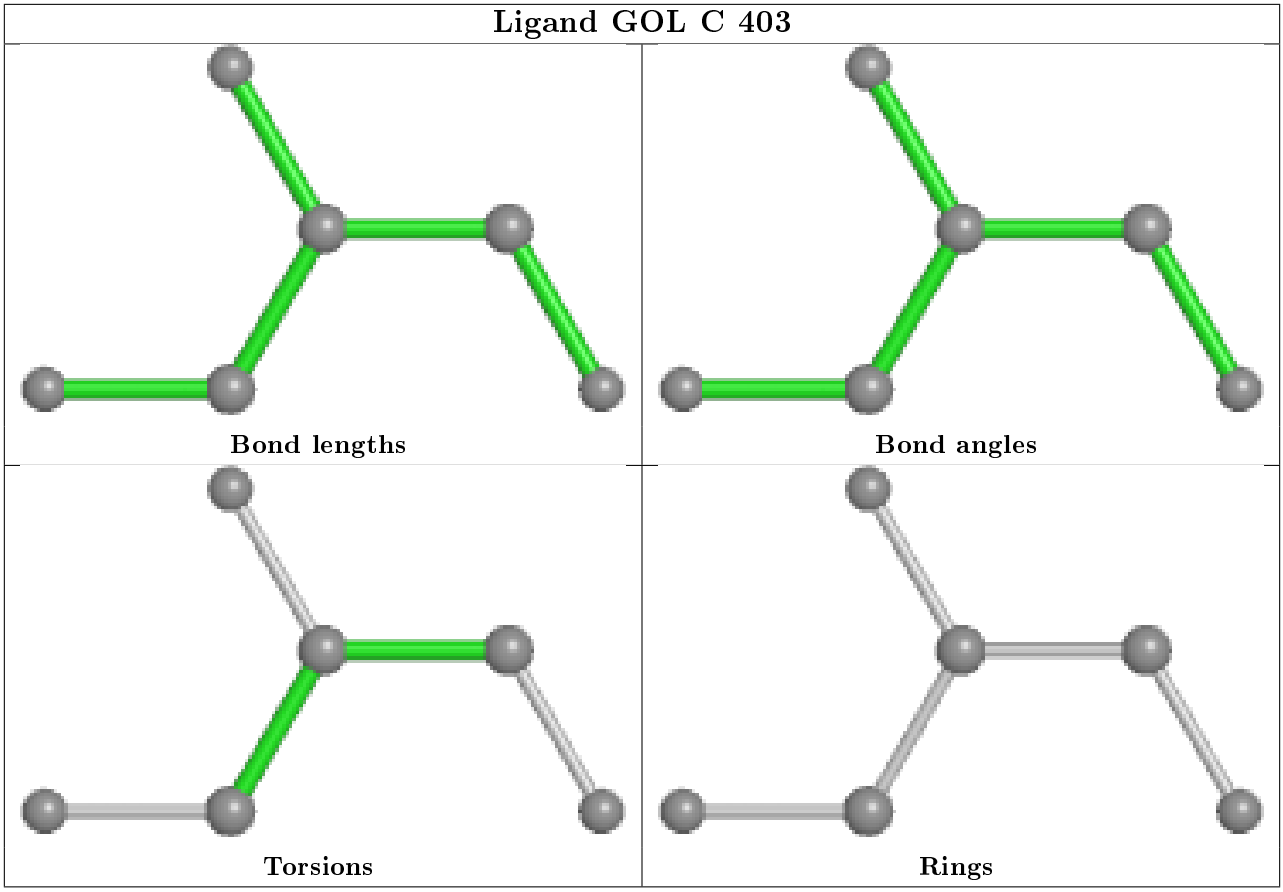
Bond angles



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	319/333 (95%)	0.05	11 (3%) 45 48	19, 26, 44, 66	0
1	B	311/333 (93%)	0.14	15 (4%) 30 32	22, 29, 46, 63	0
1	C	313/333 (93%)	-0.12	7 (2%) 62 63	15, 22, 39, 54	0
1	D	313/333 (93%)	-0.14	3 (0%) 82 83	16, 22, 36, 73	0
All	All	1256/1332 (94%)	-0.02	36 (2%) 51 54	15, 25, 43, 73	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-1	HIS	4.3
1	A	29	LYS	4.2
1	C	-1	HIS	4.1
1	B	281	ASP	3.8
1	A	30	VAL	3.8
1	B	0	HIS	3.6
1	B	56	ILE	3.6
1	A	28	GLY	3.2
1	D	0	HIS	3.0
1	B	34	ASN	3.0
1	B	240	VAL	2.9
1	A	25	TYR	2.9
1	C	110	VAL	2.9
1	A	85	ILE	2.9
1	A	0	HIS	2.8
1	B	110	VAL	2.8
1	B	78	ASP	2.6
1	C	78	ASP	2.6
1	B	119	THR	2.6
1	B	217	VAL	2.5
1	A	78	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	79	LYS	2.4
1	C	84	VAL	2.4
1	B	216	ILE	2.3
1	B	37	ASN	2.2
1	B	55	ASN	2.2
1	B	207	LYS	2.2
1	C	99	LEU	2.2
1	A	31	GLY	2.2
1	A	110	VAL	2.2
1	B	75	THR	2.2
1	A	235	GLY	2.2
1	C	132	ALA	2.1
1	C	79	LYS	2.1
1	A	106	ASP	2.1
1	D	84	VAL	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)

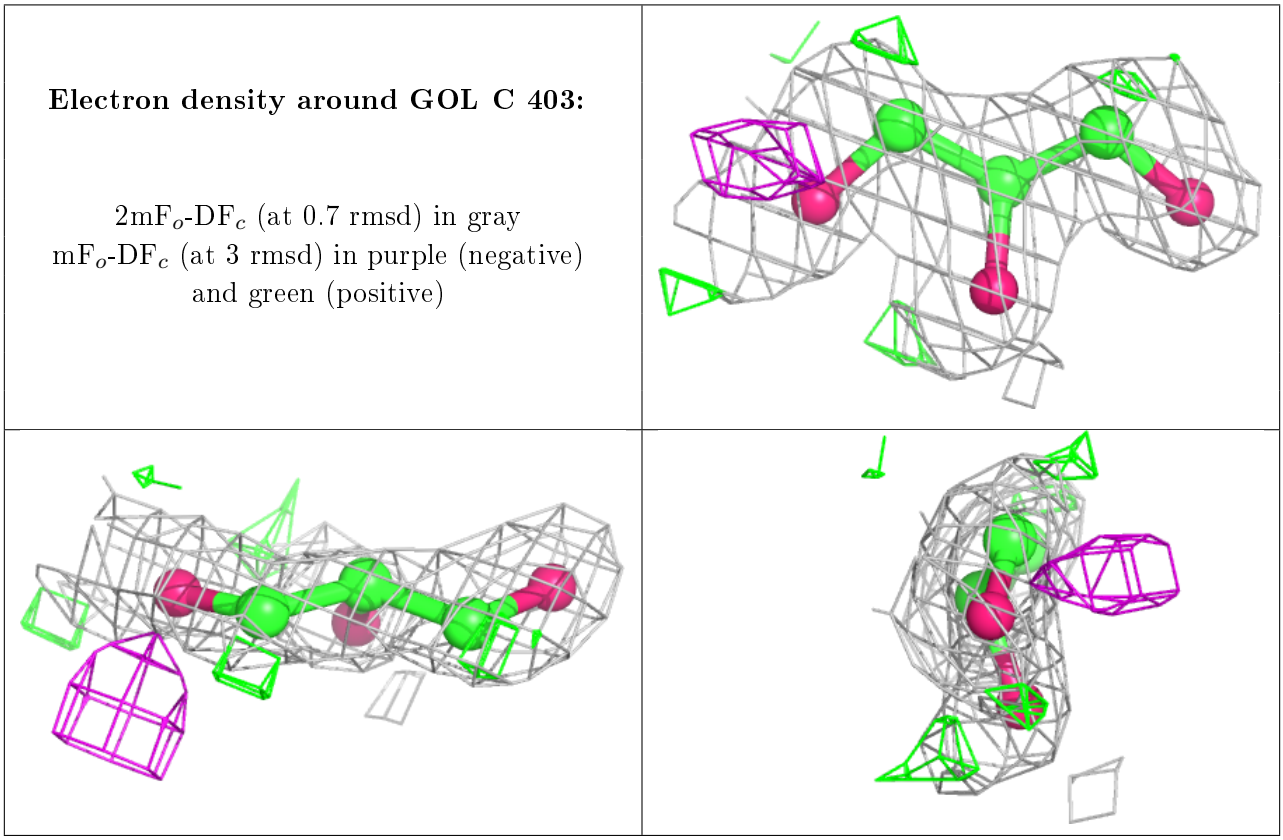
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GOL	C	403	6/6	0.78	0.25	21,22,27,37	6
4	GOL	D	501	6/6	0.86	0.15	47,49,59,59	0
4	GOL	C	402	6/6	0.88	0.14	31,42,45,47	0
2	ACY	D	502	4/4	0.88	0.12	34,35,42,45	0
2	ACY	B	401	4/4	0.88	0.12	41,42,43,55	0
2	ACY	C	401	4/4	0.89	0.10	32,42,45,46	0
3	IMD	A	402	5/5	0.91	0.17	32,35,36,39	0
2	ACY	A	401	4/4	0.94	0.12	37,38,41,43	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.

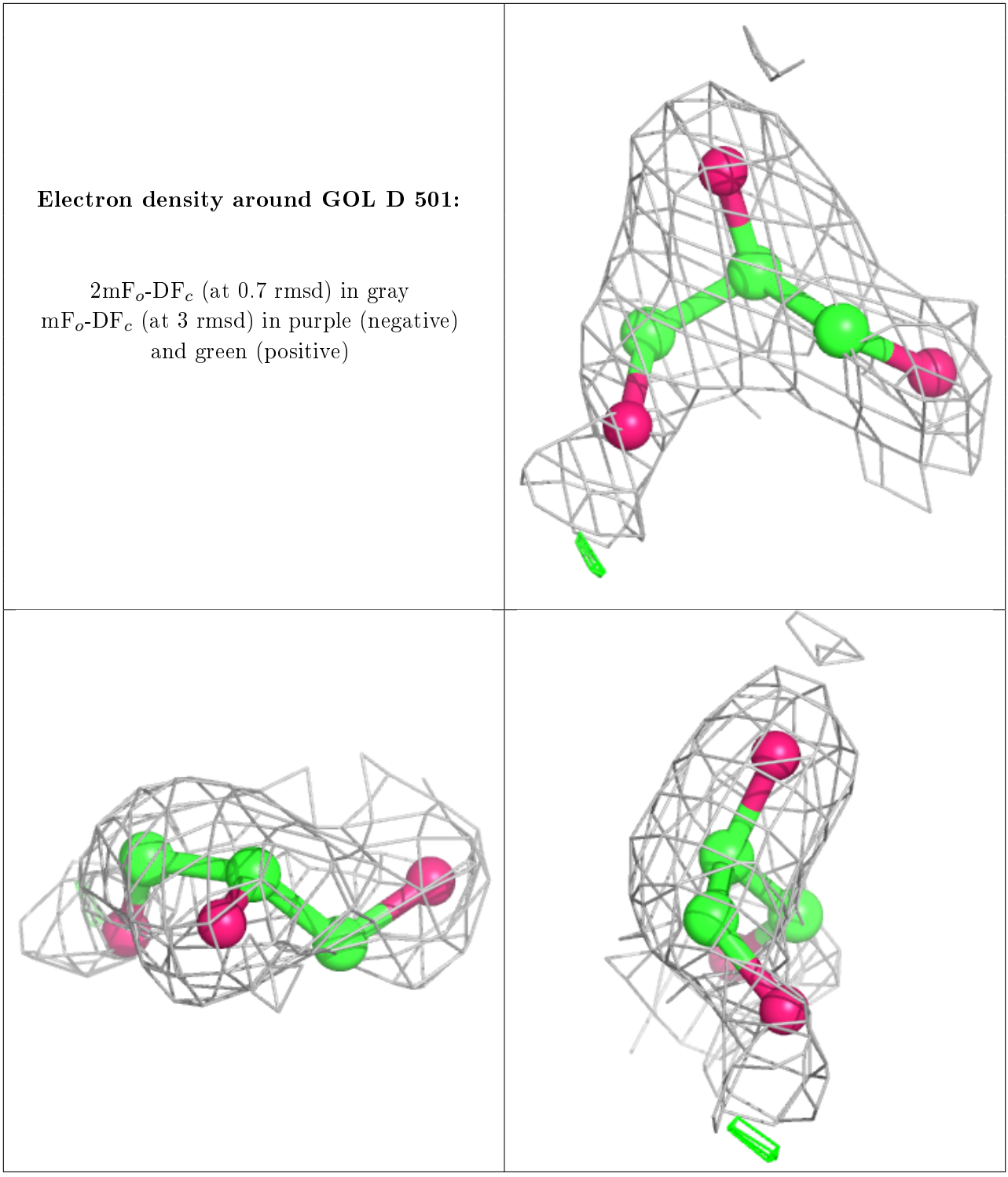
Electron density around GOL C 403:

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



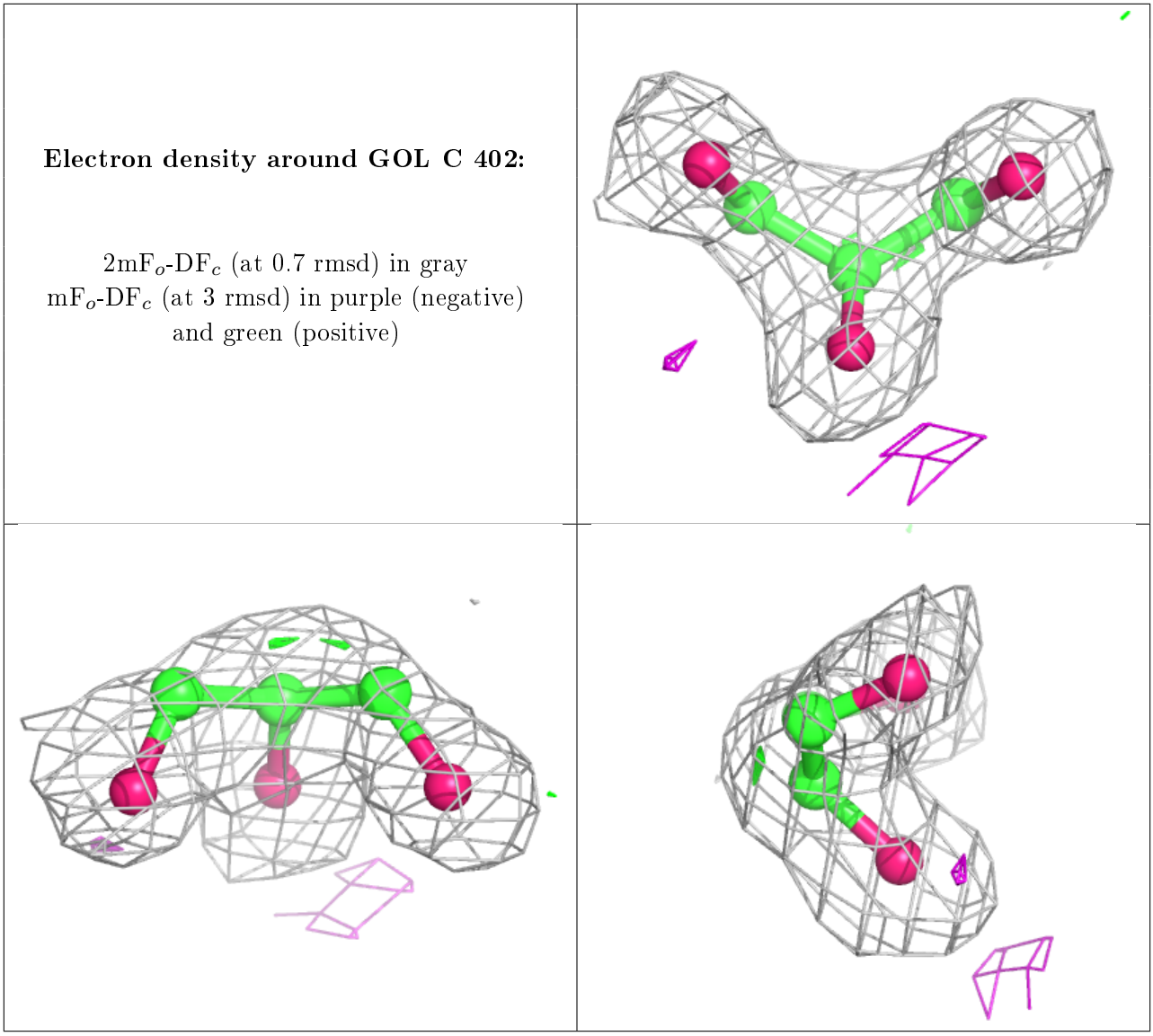
Electron density around GOL D 501:

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



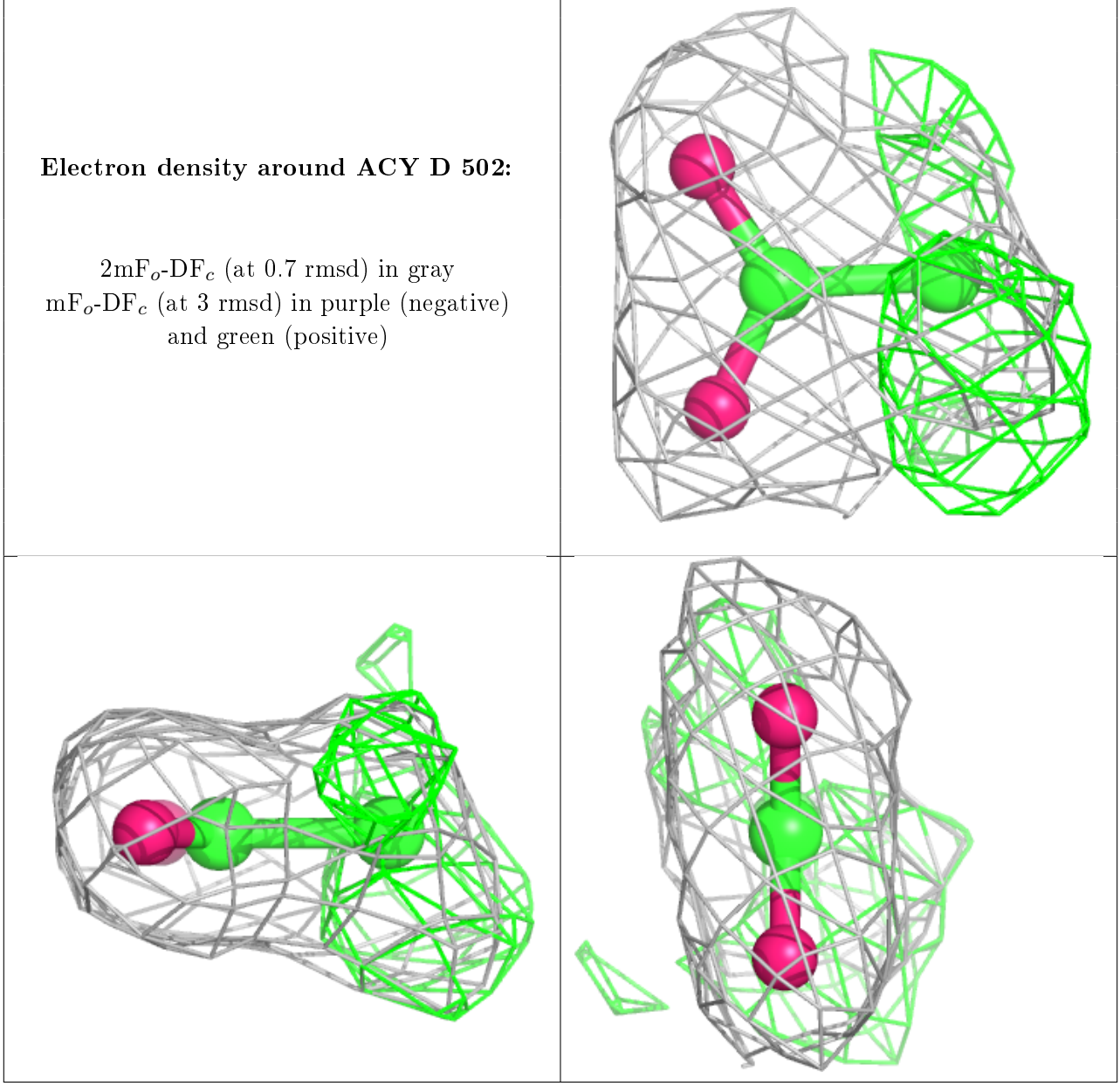
Electron density around GOL C 402:

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



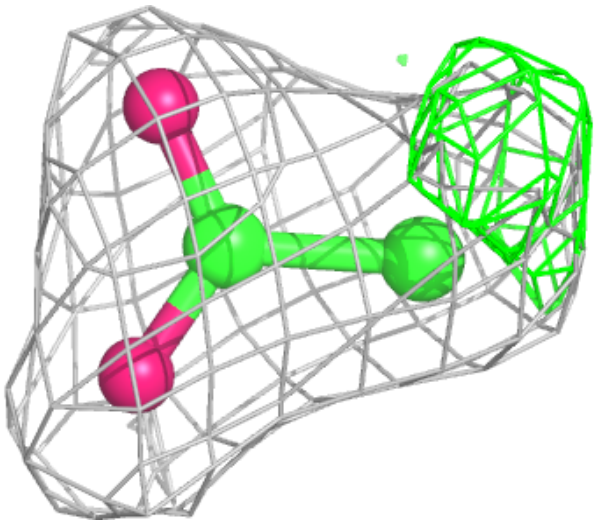
Electron density around ACY D 502:

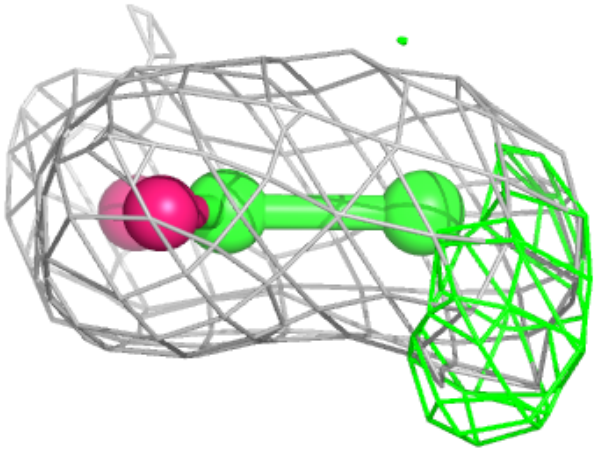
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

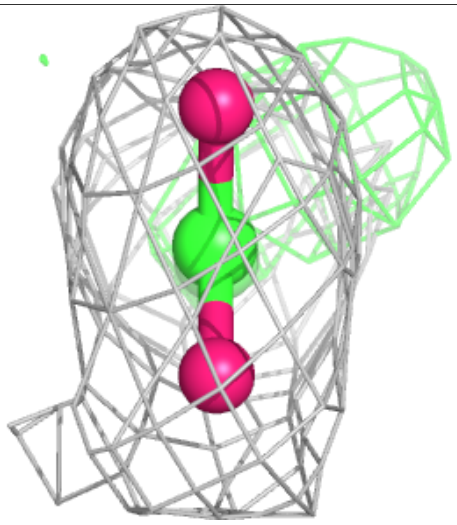


Electron density around ACY B 401:

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

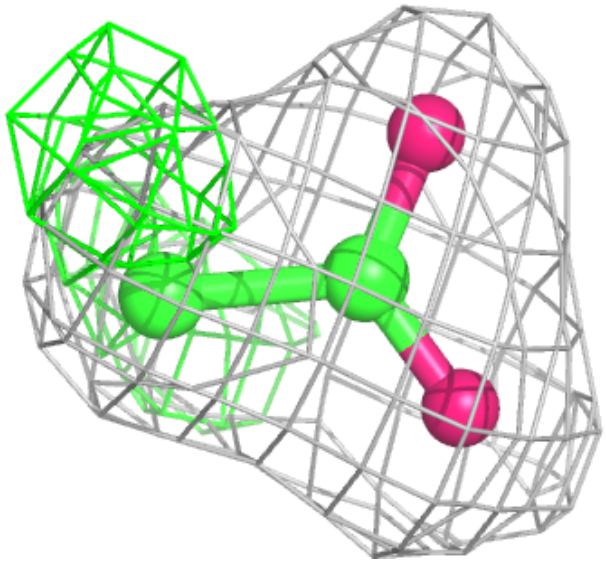


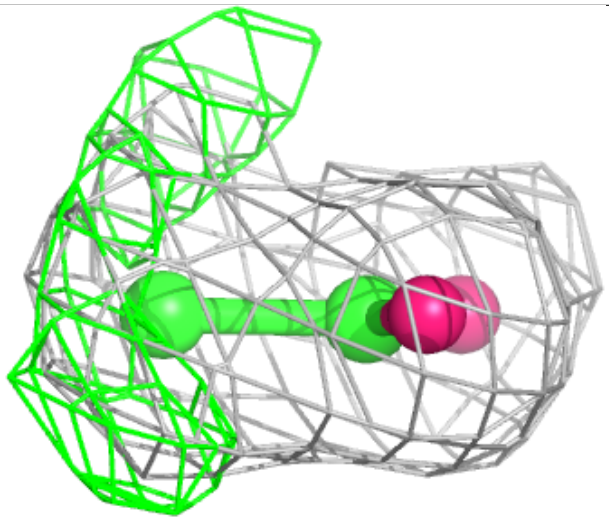


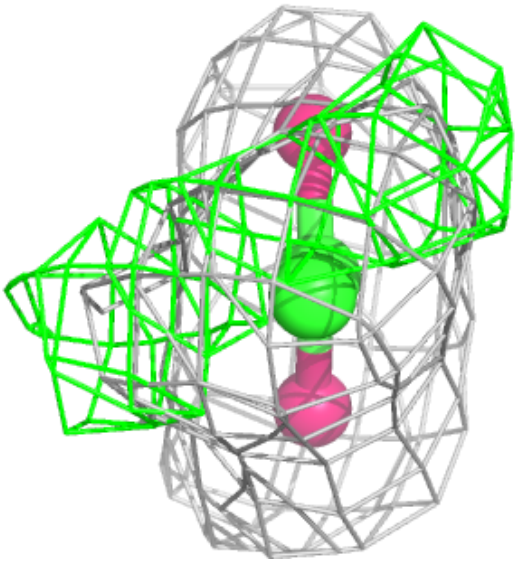


Electron density around ACY C 401:

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

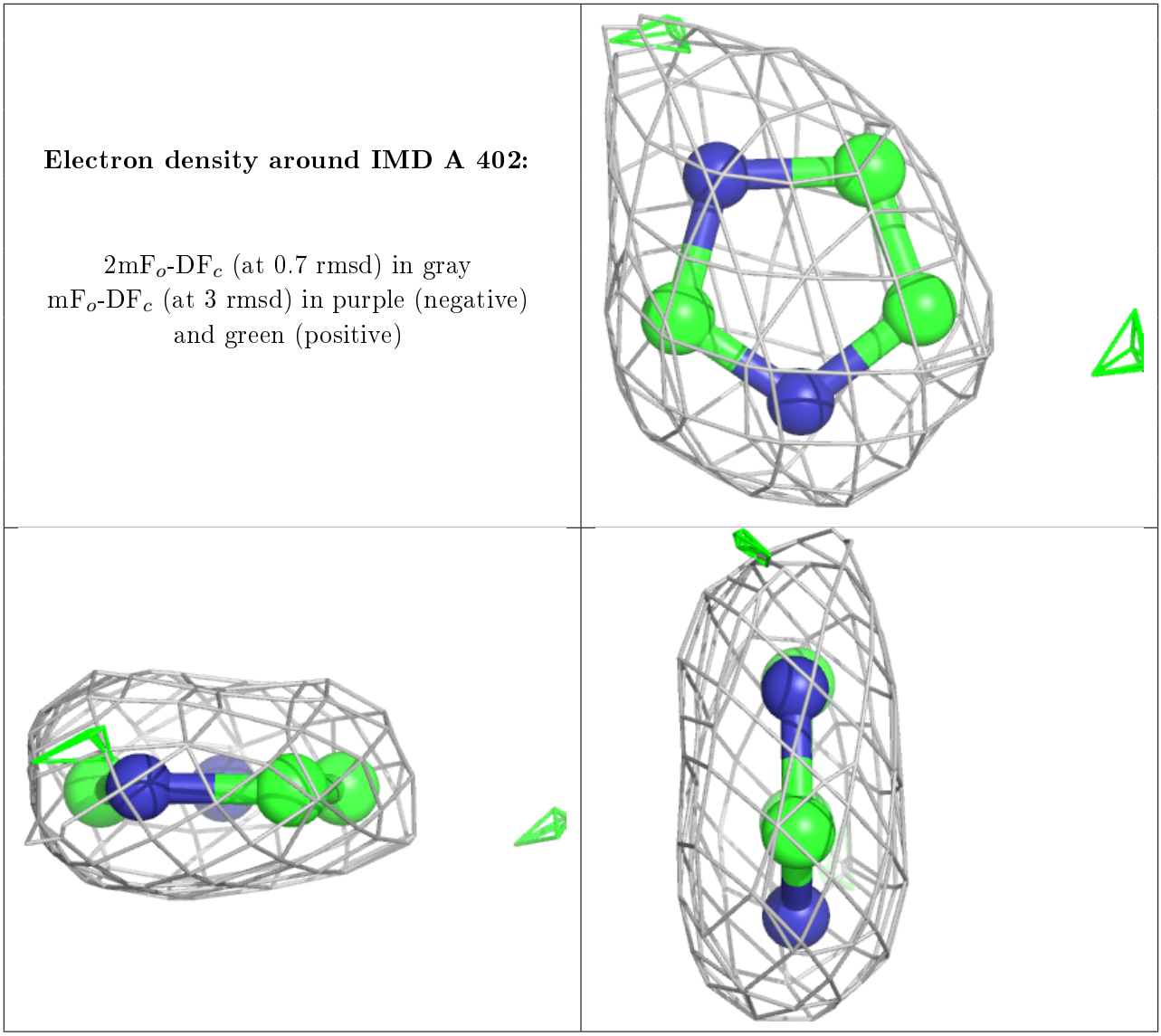






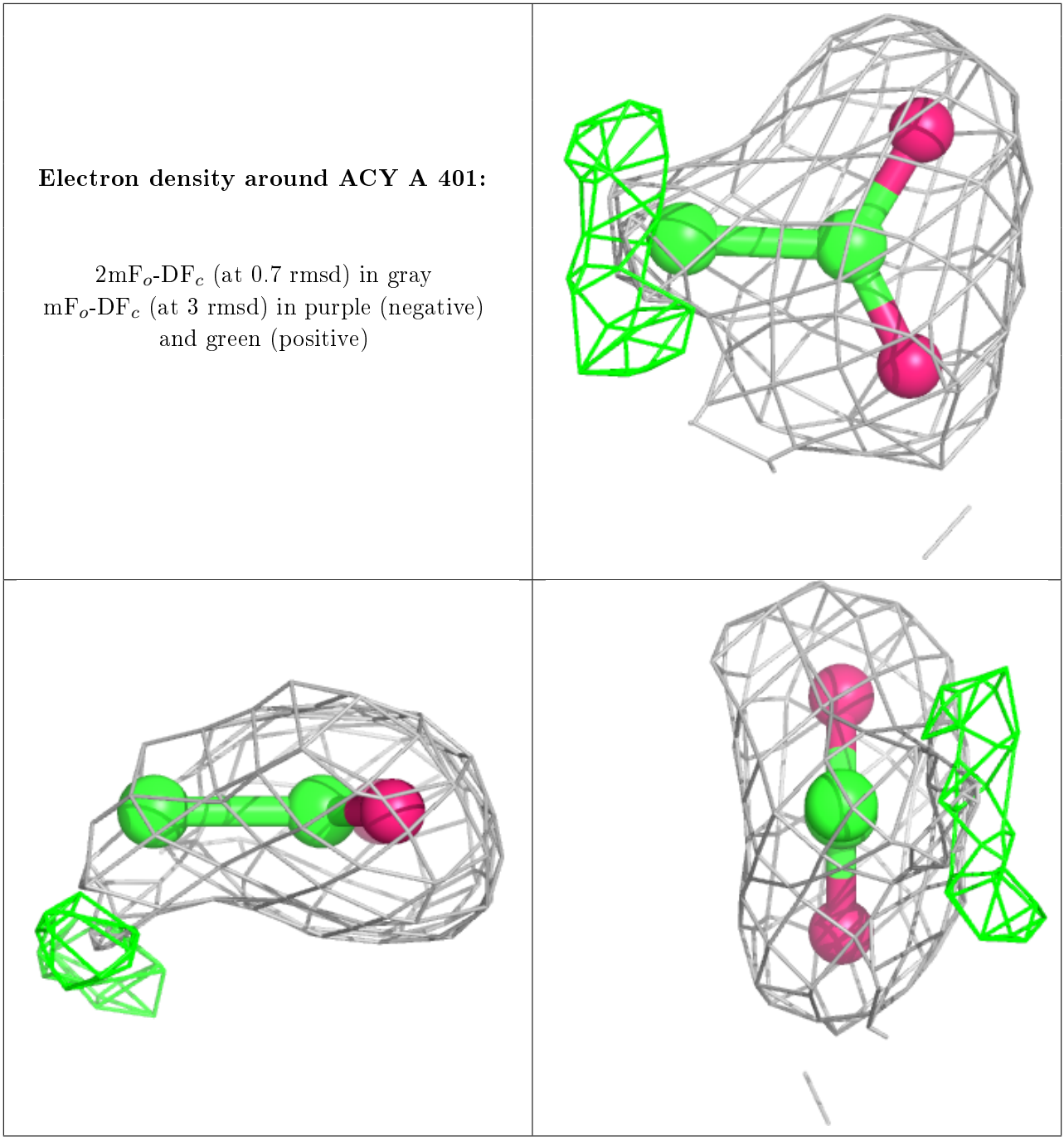
Electron density around IMD A 402:

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



Electron density around ACY A 401:

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



6.5 Other polymers

There are no such residues in this entry.