Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2025 – 12:04 PM EST

PDB ID	:	9CQ2
Title	:	CtfAB E46D active site mutant hydrolase
Authors	:	Buhrman, G.; Bing, R.
Deposited on	:	2024-07-19
Resolution	:	2.20 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:

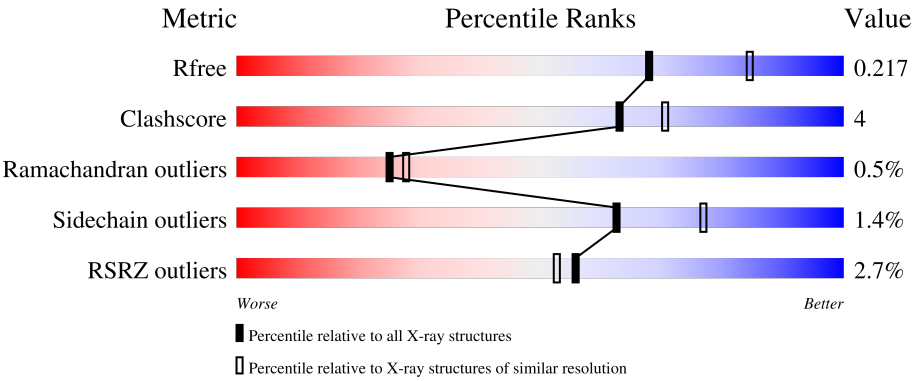
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.20 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	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	B	215	3% 88% 11%
1	C	215	5% 87% 12%
2	A	217	% 88% 10% •
2	D	217	% 87% 11% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13785 atoms, of which 6750 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 3-oxoacid CoA-transferase, B subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	214	Total	C	H	N	O	S	0	2	0
			3278	1029	1672	263	306	8			
1	C	214	Total	C	H	N	O	S	0	0	0
			3241	1018	1653	260	302	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	46	ASP	GLU	engineered mutation	UNP A6LM39
B	215	ALA	-	expression tag	UNP A6LM39
C	46	ASP	GLU	engineered mutation	UNP A6LM39
C	215	ALA	-	expression tag	UNP A6LM39

- Molecule 2 is a protein called 3-oxoacid CoA-transferase, A subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	213	Total	C	H	N	O	S	0	1	0
			3337	1033	1720	271	308	5			
2	D	213	Total	C	H	N	O	S	0	0	0
			3311	1027	1705	267	307	5			

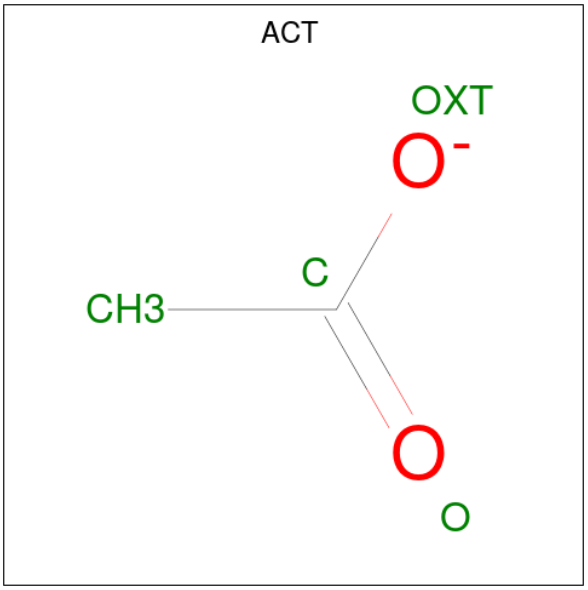
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



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

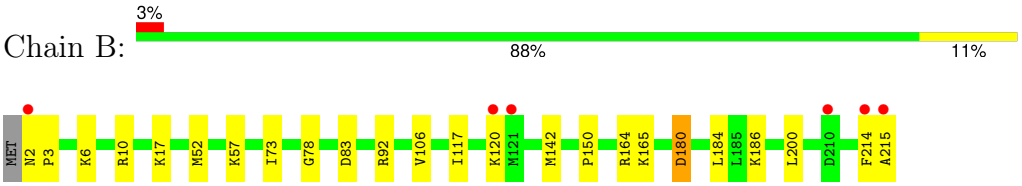
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	153	Total O 153 153	0	0
6	A	150	Total O 150 150	0	0
6	C	144	Total O 144 144	0	0
6	D	153	Total O 153 153	0	0

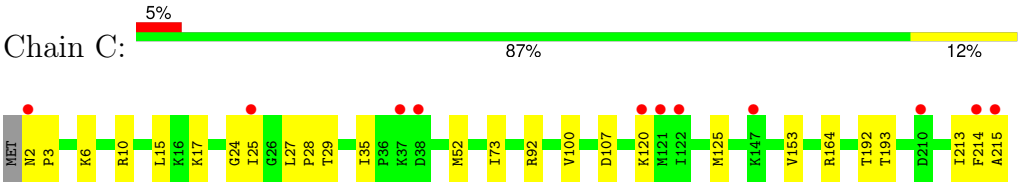
3 Residue-property plots (i)

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.

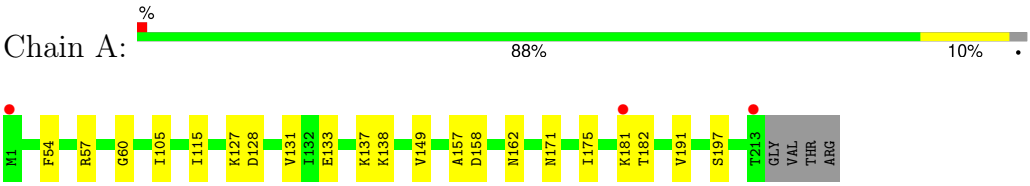
• Molecule 1: 3-oxoacid CoA-transferase, B subunit



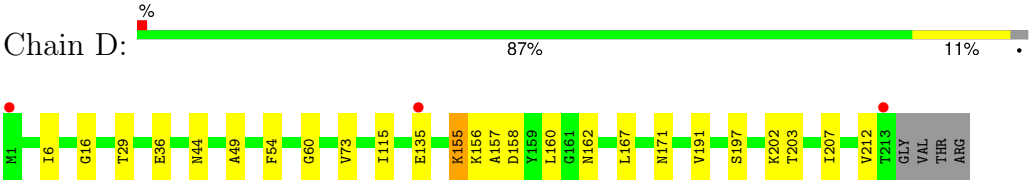
• Molecule 1: 3-oxoacid CoA-transferase, B subunit



• Molecule 2: 3-oxoacid CoA-transferase, A subunit



• Molecule 2: 3-oxoacid CoA-transferase, A subunit



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	131.37Å 131.37Å 158.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 2.20 47.19 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.19-2.20) 92.8 (47.19-2.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.169 , 0.220 0.170 , 0.217	Depositor DCC
R_{free} test set	68792 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å^2)	26.6	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13785	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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: ACT, CL, MG

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	B	0.54	0/1630	0.75	1/2207 (0.0%)
1	C	0.54	0/1612	0.72	0/2184
2	A	0.55	0/1635	0.74	0/2216
2	D	0.59	0/1624	0.76	3/2202 (0.1%)
All	All	0.55	0/6501	0.74	4/8809 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	155	LYS	CD-CE-NZ	-5.83	98.29	111.70
2	D	167	LEU	CB-CG-CD1	5.63	120.57	111.00
2	D	212	VAL	C-N-CA	5.54	135.55	121.70
1	B	83	ASP	CB-CG-OD1	5.16	122.95	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	92	ARG	Sidechain
1	C	92	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1606	1672	1670	14	0
1	C	1588	1653	1653	15	0
2	A	1617	1720	1719	11	0
2	D	1606	1705	1707	13	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	8	0	6	0	0
5	C	4	0	3	0	0
6	A	150	0	0	1	0
6	B	153	0	0	2	0
6	C	144	0	0	2	0
6	D	153	0	0	3	0
All	All	7035	6750	6758	51	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 (51) 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)
2:D:155:LYS:NZ	6:D:301:HOH:O	1.87	1.08
2:A:181:LYS:NZ	6:A:401:HOH:O	1.91	1.04
1:B:180:ASP:OD1	6:B:401:HOH:O	1.89	0.89
1:C:24:GLY:O	1:C:29:THR:HG23	1.95	0.65
2:A:115:ILE:HG22	2:D:115:ILE:HG22	1.79	0.65
2:D:135:GLU:HA	2:D:135:GLU:OE1	1.99	0.62
1:C:213:ILE:HD12	1:C:213:ILE:O	1.99	0.61
1:B:52:MET:HG3	1:B:73:ILE:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:131:VAL:HG11	2:A:138:LYS:HE3	1.84	0.60
1:C:15:LEU:HD12	1:C:35:ILE:CD1	2.34	0.58
2:D:6:ILE:HG13	2:D:36:GLU:HG3	1.87	0.56
1:C:15:LEU:HD12	1:C:35:ILE:HD13	1.88	0.55
1:C:6:LYS:HE3	1:C:215:ALA:HA	1.88	0.55
1:B:52:MET:HG3	1:B:73:ILE:CD1	2.37	0.55
1:C:28:PRO:HB3	1:C:100:VAL:HG12	1.92	0.52
2:D:202:LYS:HD2	6:D:377:HOH:O	2.08	0.52
1:B:6:LYS:HE3	1:B:215:ALA:HA	1.93	0.51
2:D:54:PHE:O	2:D:60:GLY:HA3	2.11	0.50
2:D:16:GLY:HA2	2:D:44:ASN:O	2.11	0.50
1:C:192:THR:HG23	1:C:193:THR:N	2.27	0.49
2:A:54:PHE:O	2:A:60:GLY:HA3	2.13	0.48
1:C:10:ARG:HB2	1:C:215:ALA:CB	2.44	0.48
2:A:158:ASP:HA	2:A:191:VAL:O	2.13	0.47
1:C:52:MET:HG3	1:C:73:ILE:HD12	1.97	0.46
1:B:10:ARG:HB2	1:B:215:ALA:CB	2.46	0.46
2:A:133:GLU:HA	2:A:137:LYS:O	2.15	0.46
1:B:106:VAL:HG23	1:B:142:MET:CE	2.46	0.45
2:A:54:PHE:HD1	2:A:57:ARG:HD2	1.80	0.45
2:A:105:ILE:HG22	2:A:175:ILE:HG22	1.98	0.45
1:B:57:LYS:NZ	6:B:404:HOH:O	2.46	0.45
1:C:17:LYS:HE3	6:C:462:HOH:O	2.17	0.45
1:B:10:ARG:HB2	1:B:215:ALA:HB3	1.99	0.44
2:D:157:ALA:HA	2:D:162:ASN:O	2.17	0.44
1:B:117:ILE:CG2	1:B:120:LYS:HD2	2.47	0.44
1:B:78:GLY:HA3	2:D:160:LEU:HD12	1.99	0.44
1:B:2:ASN:N	1:B:3:PRO:HD2	2.33	0.44
2:D:49:ALA:O	2:D:73:VAL:HA	2.18	0.43
1:B:150:PRO:HB3	1:B:200:LEU:O	2.18	0.43
2:D:156:LYS:HE3	6:D:362:HOH:O	2.18	0.43
1:C:2:ASN:N	1:C:3:PRO:HD2	2.33	0.43
1:C:107:ASP:HA	1:C:153:VAL:O	2.19	0.42
1:C:27:LEU:O	1:C:27:LEU:HD23	2.19	0.42
2:A:157:ALA:HA	2:A:162:ASN:O	2.20	0.42
2:D:158:ASP:HA	2:D:191:VAL:O	2.19	0.42
2:A:149:VAL:HA	2:A:182:THR:O	2.20	0.41
1:C:25:ILE:HD12	6:C:490:HOH:O	2.19	0.41
1:B:184:LEU:HD23	1:B:186:LYS:HD3	2.01	0.41
1:B:10:ARG:CG	1:B:215:ALA:HB3	2.52	0.41
2:A:127:LYS:HE2	2:A:128:ASP:OD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LEU:HB3	1:C:28:PRO:HD3	2.03	0.40
2:D:203:THR:HG23	2:D:207:ILE:HD11	2.02	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	B	214/215 (100%)	209 (98%)	4 (2%)	1 (0%)	25	28
1	C	212/215 (99%)	205 (97%)	6 (3%)	1 (0%)	25	28
2	A	212/217 (98%)	208 (98%)	3 (1%)	1 (0%)	25	28
2	D	211/217 (97%)	207 (98%)	3 (1%)	1 (0%)	25	28
All	All	849/864 (98%)	829 (98%)	16 (2%)	4 (0%)	25	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	214	PHE
1	C	214	PHE
2	D	171	ASN
2	A	171	ASN

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	B	173/175 (99%)	168 (97%)	5 (3%)	37	50
1	C	171/175 (98%)	168 (98%)	3 (2%)	54	69
2	A	179/181 (99%)	178 (99%)	1 (1%)	84	91
2	D	178/181 (98%)	176 (99%)	2 (1%)	70	82
All	All	701/712 (98%)	690 (98%)	11 (2%)	62	73

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

Mol	Chain	Res	Type
1	B	17	LYS
1	B	164	ARG
1	B	165[A]	LYS
1	B	165[B]	LYS
1	B	180	ASP
2	A	197	SER
1	C	120	LYS
1	C	125	MET
1	C	164	ARG
2	D	29	THR
2	D	197	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
5	ACT	A	302	-	3,3,3	2.70	2 (66%)	3,3,3	1.29	0
5	ACT	C	301	-	3,3,3	1.48	1 (33%)	3,3,3	1.11	0
5	ACT	A	301	-	3,3,3	1.26	0	3,3,3	1.88	2 (66%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	302	ACT	CH3-C	3.76	1.63	1.49
5	A	302	ACT	O-C	2.78	1.34	1.22
5	C	301	ACT	CH3-C	2.05	1.57	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	301	ACT	OXT-C-O	2.35	130.74	122.03
5	A	301	ACT	O-C-CH3	-2.26	113.26	122.53

There are no chirality outliers.

There are no torsion outliers.

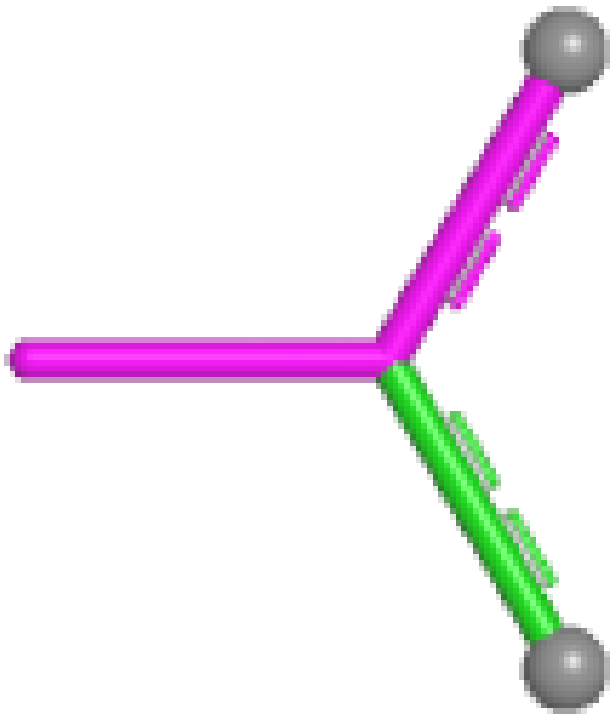
There are no ring outliers.

No monomer is involved in short contacts.

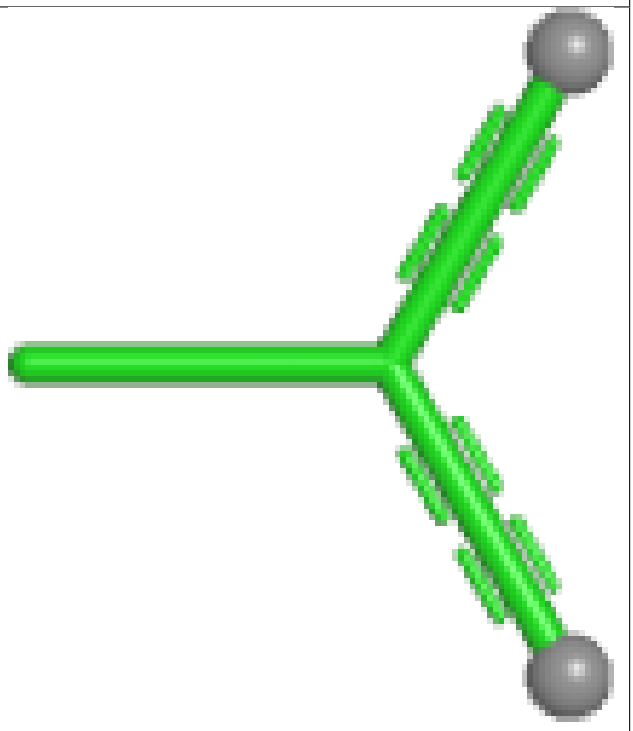
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

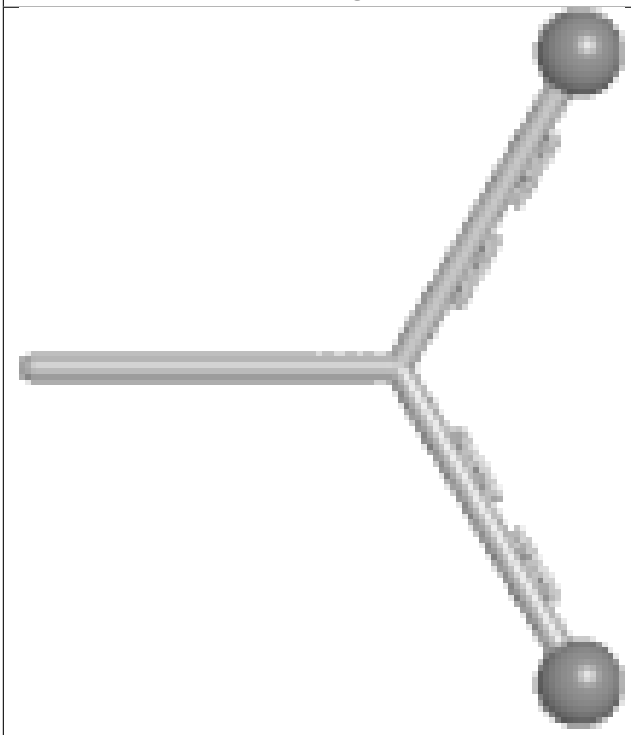
Ligand ACT A 302



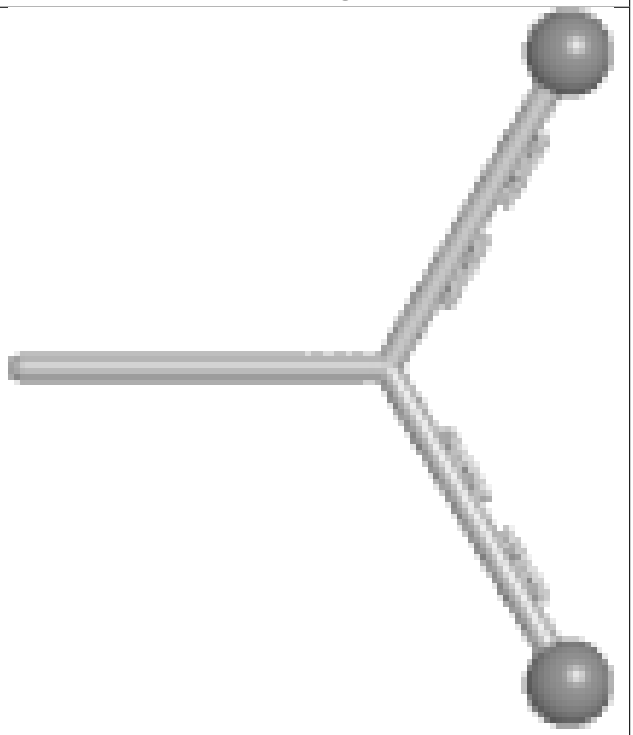
Bond lengths



Bond angles

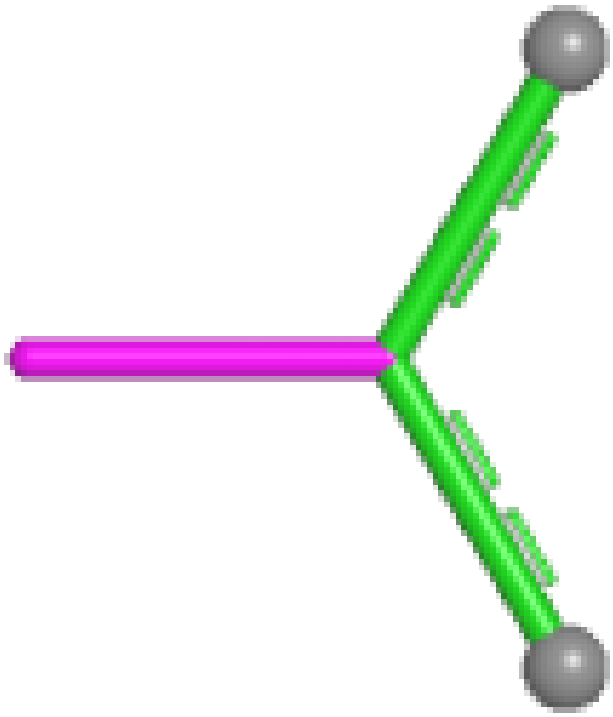


Torsions

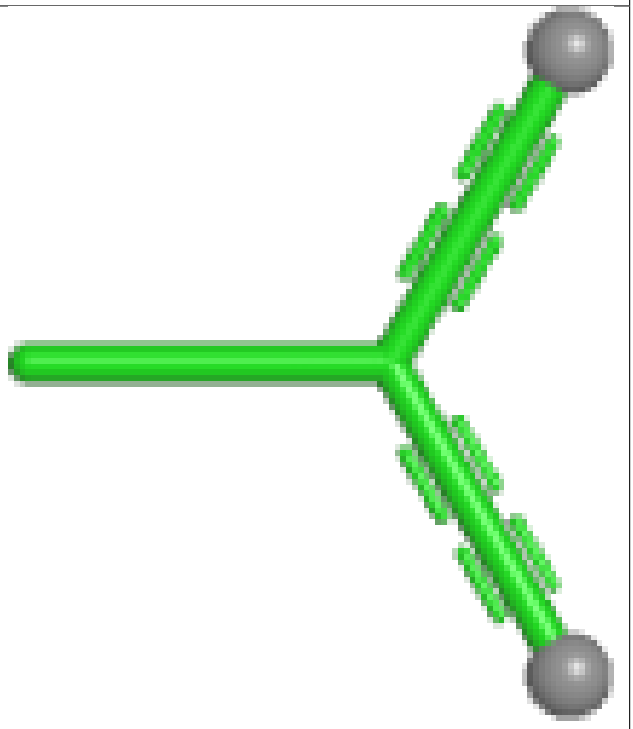


Rings

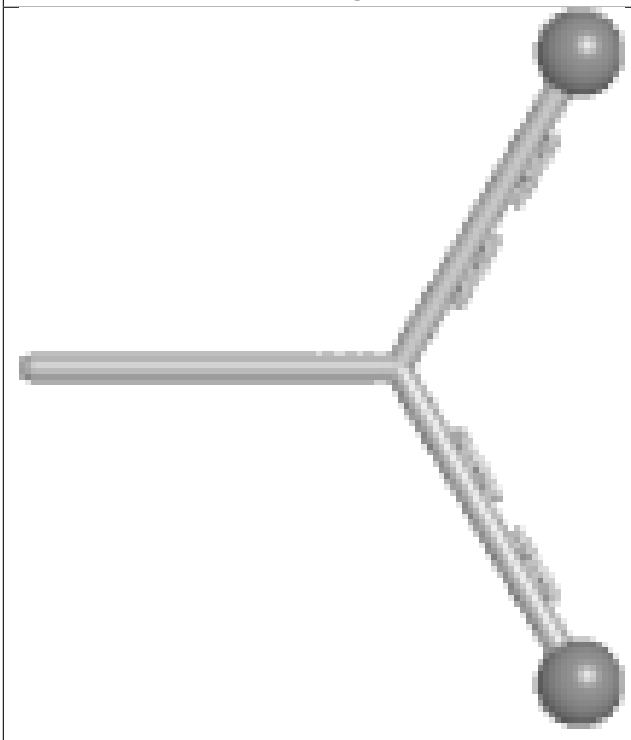
Ligand ACT C 301



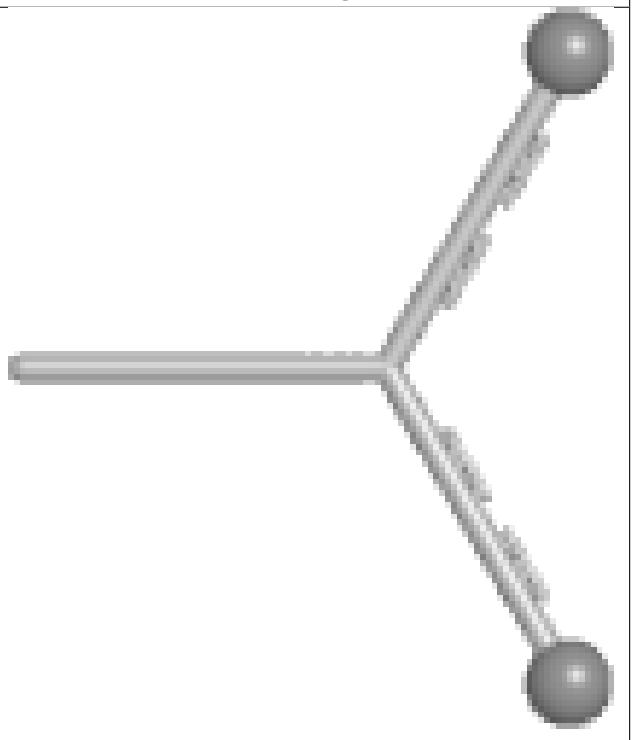
Bond lengths



Bond angles

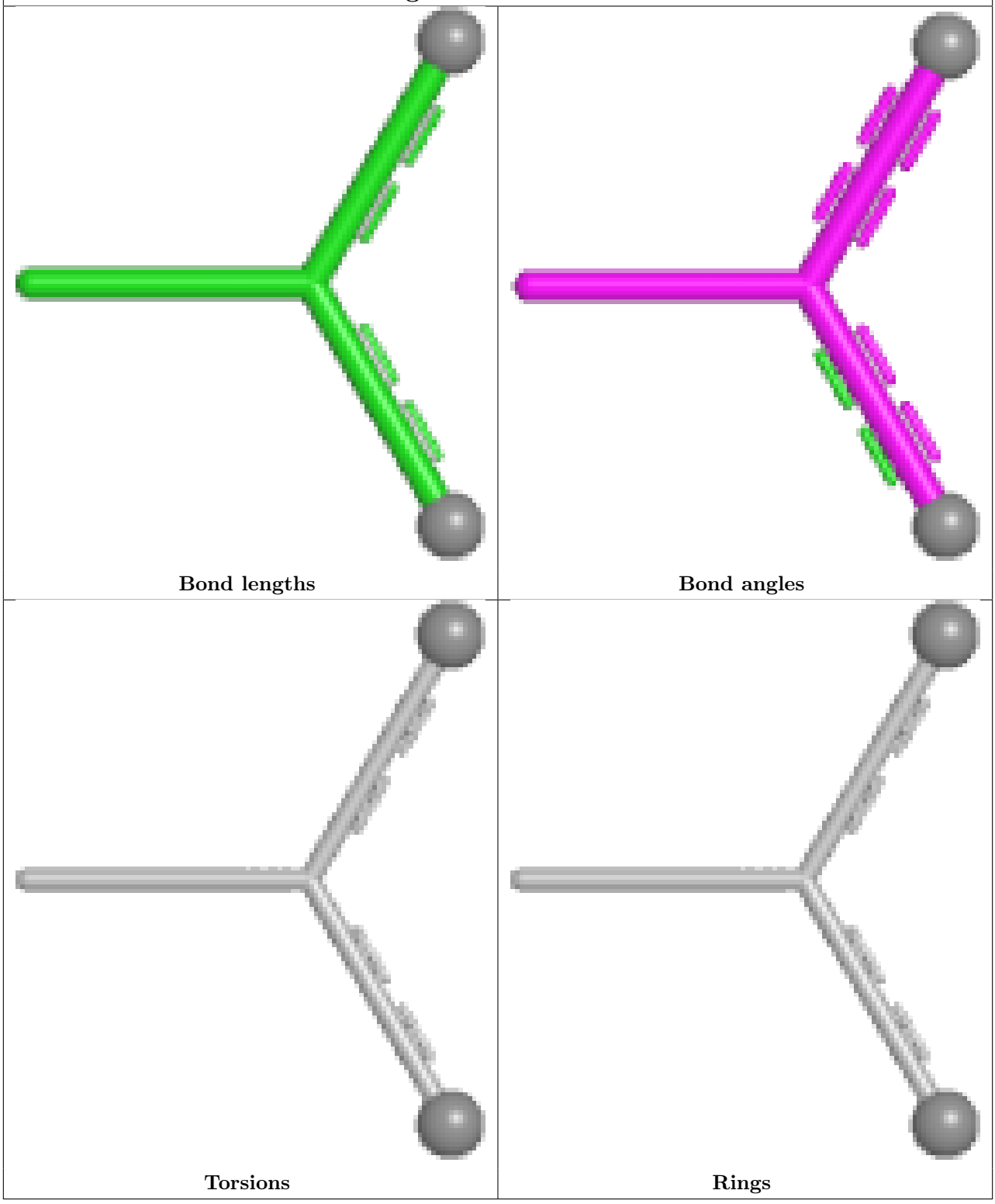


Torsions



Rings

Ligand ACT A 301



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	B	214/215 (99%)	-0.32	6 (2%)	55	52	17, 37, 77, 125	2 (0%)
1	C	214/215 (99%)	-0.28	11 (5%)	34	31	18, 38, 78, 133	0
2	A	213/217 (98%)	-0.71	3 (1%)	73	70	18, 30, 68, 109	1 (0%)
2	D	213/217 (98%)	-0.65	3 (1%)	73	70	18, 31, 67, 107	0
All	All	854/864 (98%)	-0.49	23 (2%)	56	53	17, 34, 75, 133	3 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	PHE	5.0
1	C	121	MET	4.7
1	C	214	PHE	4.3
2	D	213	THR	4.1
2	A	213	THR	4.0
1	B	210	ASP	3.5
2	A	1	MET	3.5
1	C	215	ALA	3.4
1	C	147	LYS	3.2
1	B	121	MET	2.9
1	B	215	ALA	2.8
1	C	25	ILE	2.7
1	C	2	ASN	2.5
2	D	135	GLU	2.3
1	C	120	LYS	2.3
1	C	210	ASP	2.3
2	A	181	LYS	2.3
1	C	122	ILE	2.3
2	D	1	MET	2.2
1	C	37	LYS	2.2
1	B	120	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2	ASN	2.0
1	C	38	ASP	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)

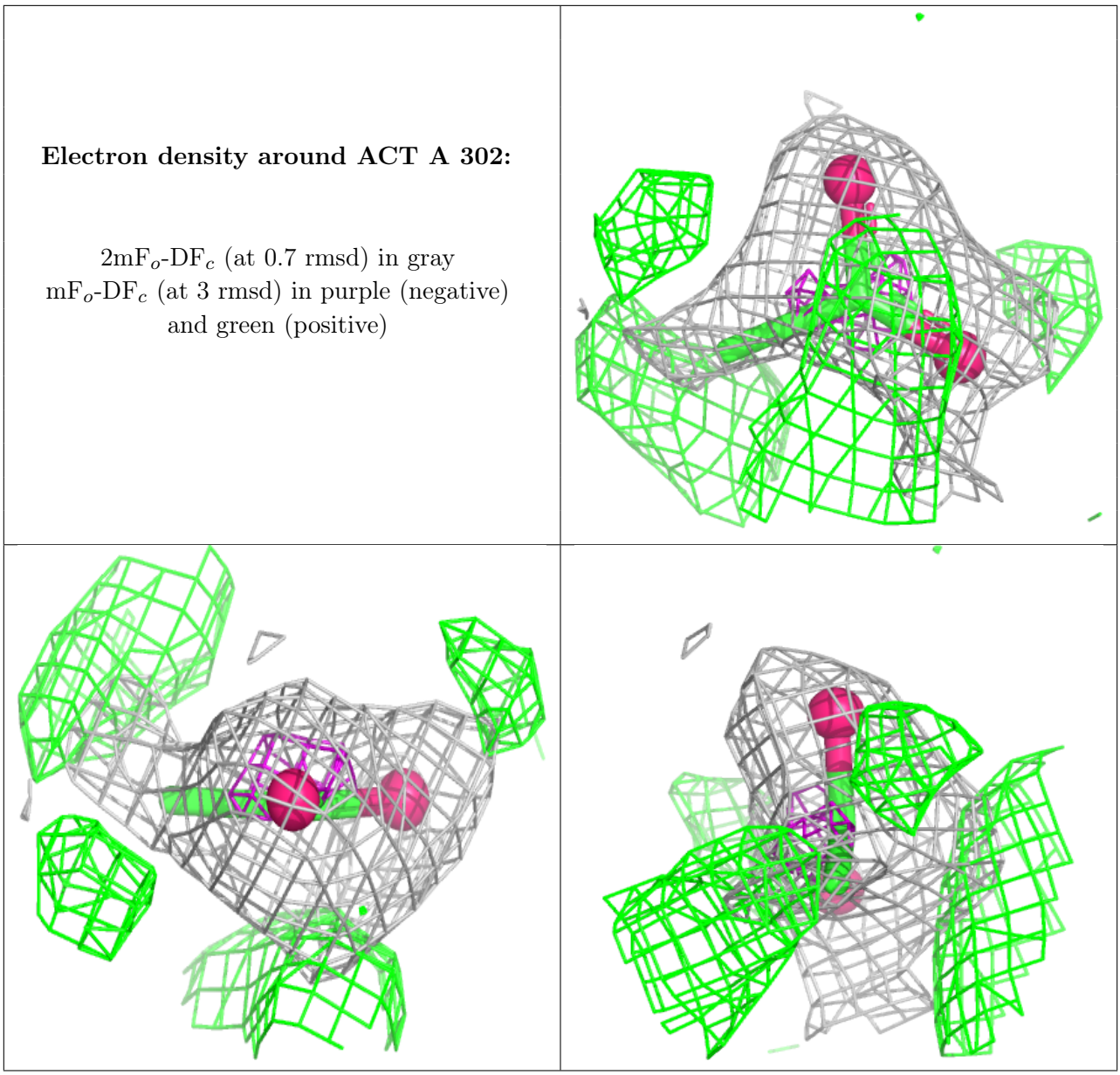
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	MG	B	301	1/1	0.65	0.36	129,129,129,129	0
5	ACT	A	302	4/4	0.80	0.22	35,43,44,45	0
5	ACT	C	301	4/4	0.84	0.21	43,44,50,60	0
4	CL	B	303	1/1	0.85	0.45	98,98,98,98	0
4	CL	C	303	1/1	0.90	0.17	61,61,61,61	0
5	ACT	A	301	4/4	0.93	0.14	42,46,48,54	0
4	CL	C	302	1/1	0.93	0.14	67,67,67,67	0
3	MG	B	302	1/1	0.93	0.12	63,63,63,63	0
3	MG	A	303	1/1	0.94	0.08	38,38,38,38	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.

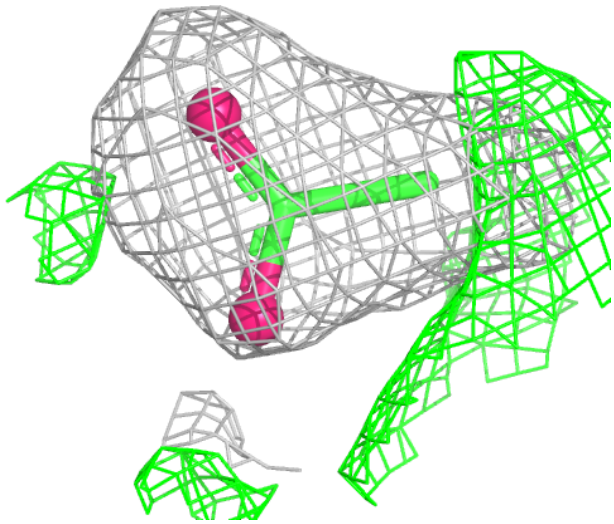
Electron density around ACT A 302:

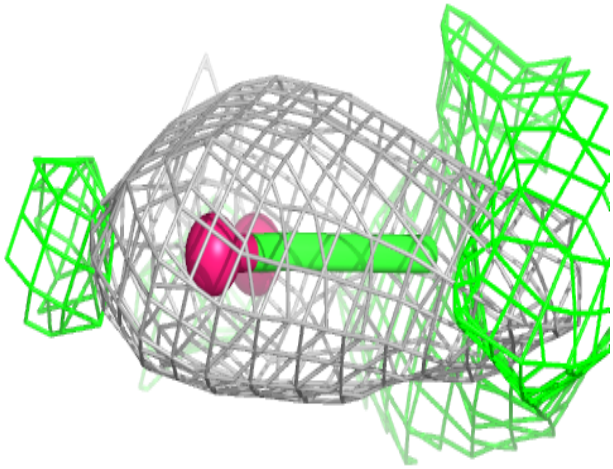
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

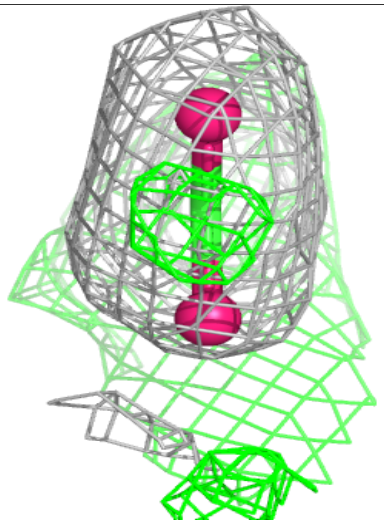


Electron density around ACT C 301:

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

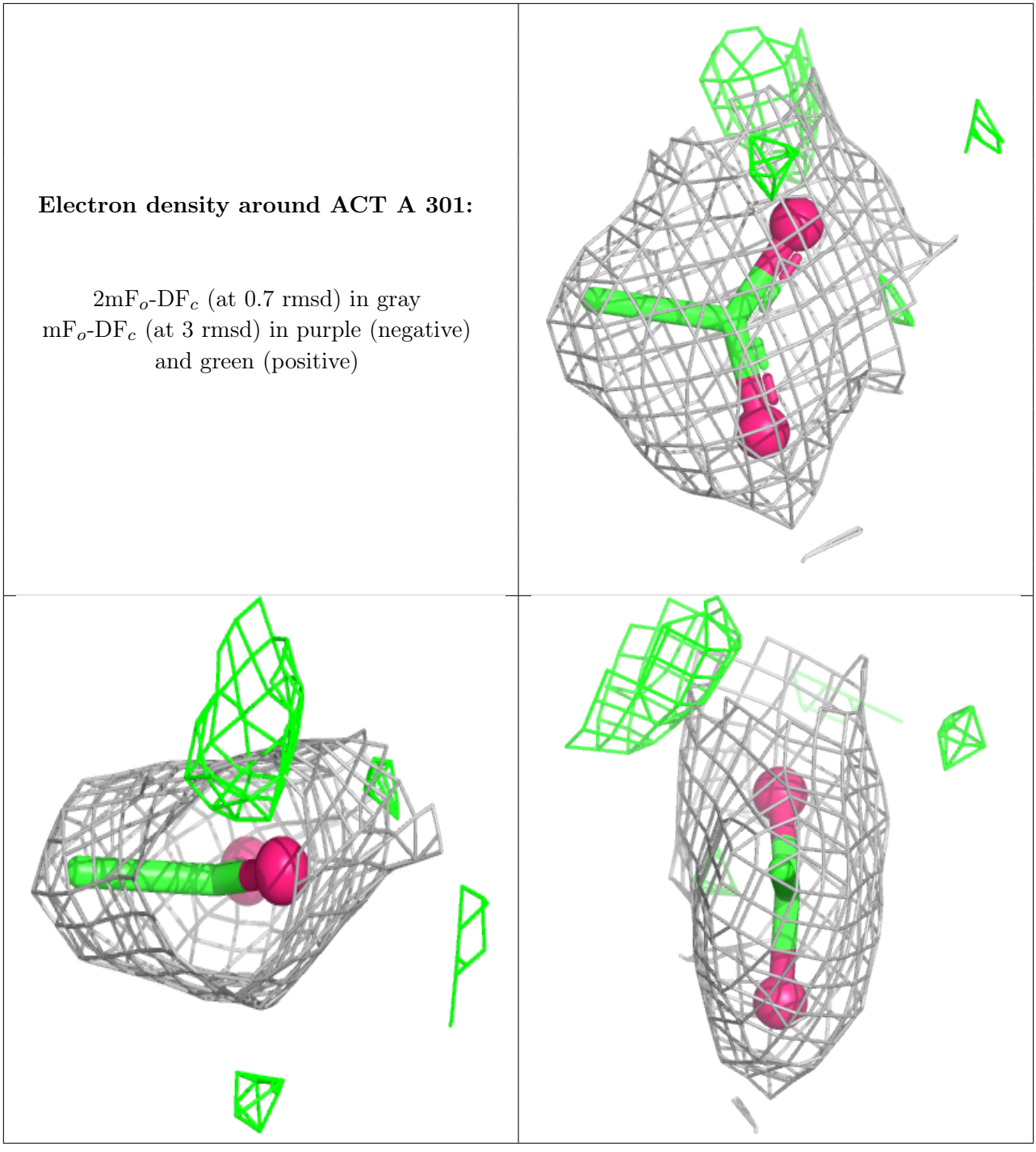






Electron density around ACT A 301:

$2mF_o$-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.