Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2025 – 12:05 PM EST

PDB ID	:	9CTD
Title	:	CtfAB F42TS45C mutant co-crystallized with acetyl-CoA
Authors	:	Buhrman, G.; Bing, R.
Deposited on	:	2024-07-24
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:

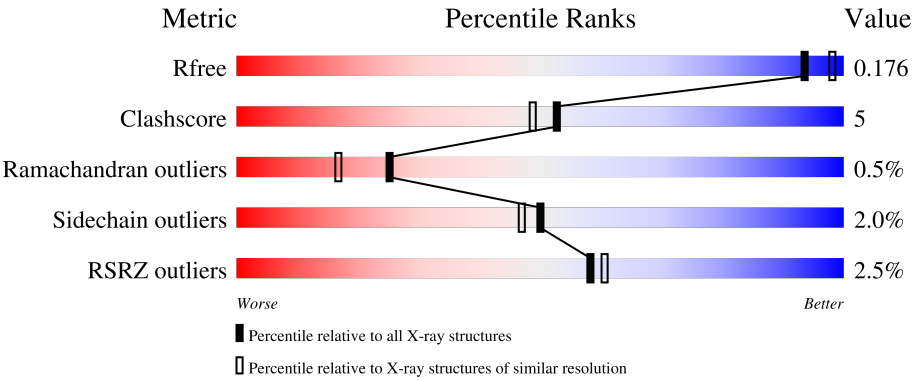
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (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 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	217	90% 8%
1	D	217	88% 10%
2	B	215	4% 89% 10%
2	C	215	4% 86% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	A	303	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14161 atoms, of which 6907 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, A subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	213	Total	C	H	N	O	S	0	1	0
			3324	1030	1712	268	309	5			
1	A	213	Total	C	H	N	O	S	0	3	0
			3362	1040	1731	274	312	5			

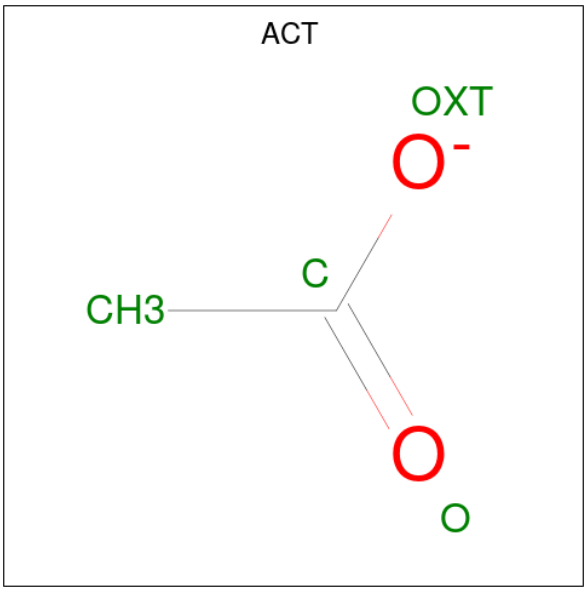
- Molecule 2 is a protein called 3-oxoacid CoA-transferase, B subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	214	Total	C	H	N	O	S	0	1	0
			3285	1025	1683	264	304	9			
2	B	214	Total	C	H	N	O	S	0	0	0
			3269	1020	1676	262	302	9			

There are 6 discrepancies between the modelled and reference sequences:

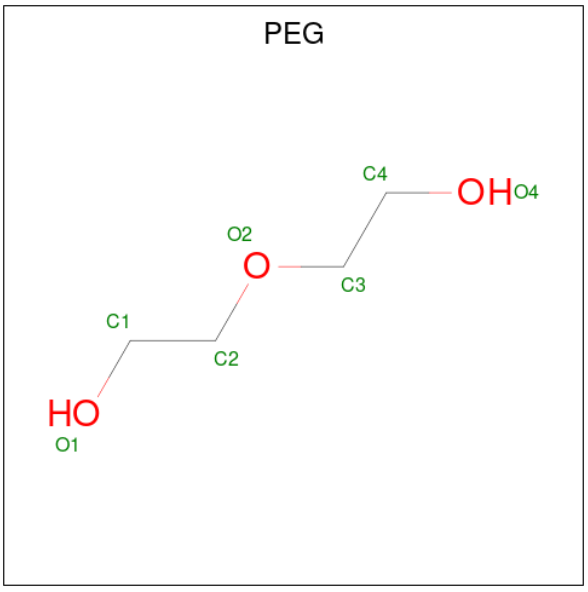
Chain	Residue	Modelled	Actual	Comment	Reference
C	42	THR	PHE	engineered mutation	UNP A6LM39
C	45	CYS	SER	engineered mutation	UNP A6LM39
C	215	ALA	-	expression tag	UNP A6LM39
B	42	THR	PHE	engineered mutation	UNP A6LM39
B	45	CYS	SER	engineered mutation	UNP A6LM39
B	215	ALA	-	expression tag	UNP A6LM39

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



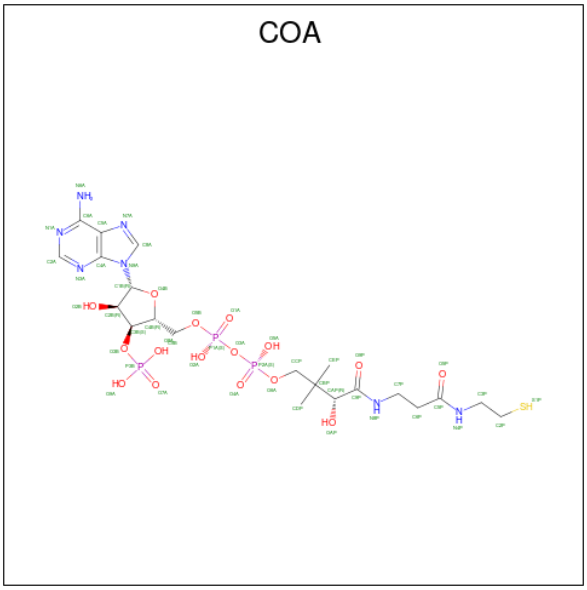
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			17	4	10	3		
4	D	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			9	2	5	2		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	A	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	C	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		
4	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			37	15	5	14	3		
5	B	1	Total	C	N	O	P	0	0
			37	15	5	14	3		

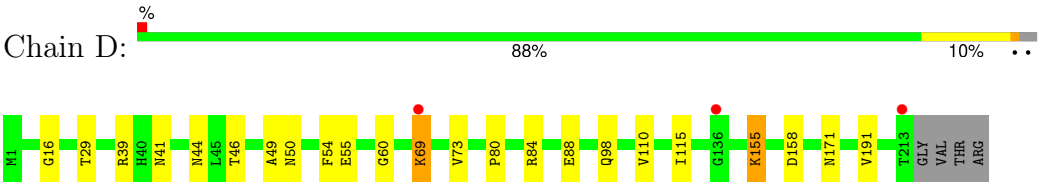
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	167	Total	O	0	0
			167	167		
6	A	174	Total	O	0	0
			174	174		
6	C	167	Total	O	0	0
			167	167		
6	B	144	Total	O	0	0
			144	144		

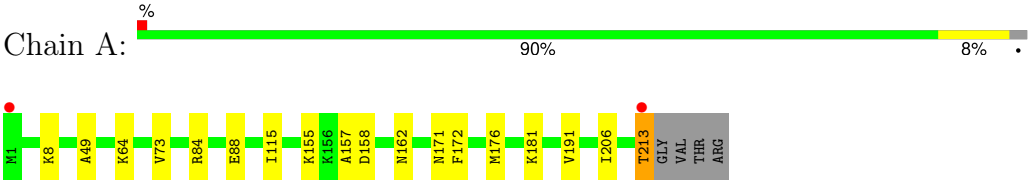
3 Residue-property plots (i)

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.

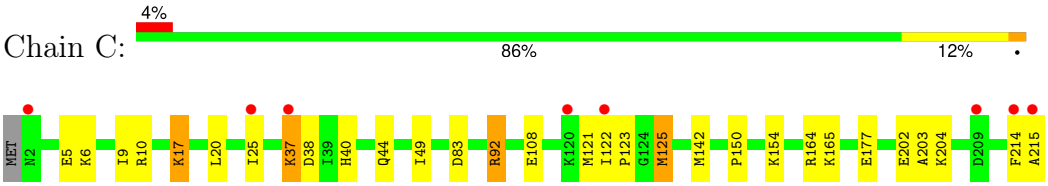
• Molecule 1: 3-oxoacid CoA-transferase, A subunit



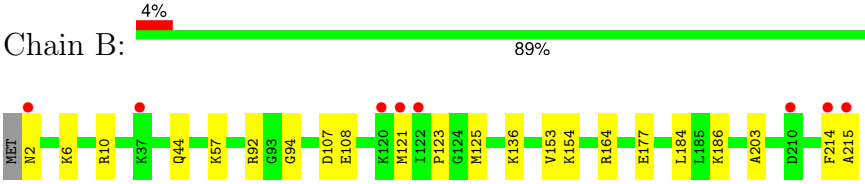
• Molecule 1: 3-oxoacid CoA-transferase, A subunit



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



• Molecule 2: 3-oxoacid CoA-transferase, B 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	130.69Å 130.69Å 155.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.95 – 1.90 41.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.7 (41.95-1.90) 97.5 (41.95-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.151 , 0.177 0.151 , 0.176	Depositor DCC
R_{free} test set	103976 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 42.1	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	14161	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 3.58% 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: COA, ACT, PEG

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	0.57	0/1649	0.74	1/2236 (0.0%)
1	D	0.54	0/1630	0.74	1/2211 (0.0%)
2	B	0.52	0/1616	0.72	1/2187 (0.0%)
2	C	0.53	0/1625	0.77	5/2199 (0.2%)
All	All	0.54	0/6520	0.74	8/8833 (0.1%)

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
2	C	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	69	LYS	CD-CE-NZ	-9.95	88.81	111.70
2	C	142	MET	CB-CA-C	-5.69	99.02	110.40
1	A	213	THR	CA-CB-CG2	5.54	120.16	112.40
2	C	142	MET	N-CA-CB	5.25	120.05	110.60
2	C	125	MET	CA-CB-CG	5.15	122.06	113.30
2	C	92	ARG	NE-CZ-NH1	5.09	122.85	120.30
2	B	57	LYS	CA-CB-CG	-5.06	102.27	113.40
2	C	83	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	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	A	1631	1731	1729	13	0
1	D	1612	1712	1712	13	0
2	B	1593	1676	1675	18	0
2	C	1602	1683	1682	22	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
4	A	25	35	35	4	0
4	B	14	20	20	2	0
4	C	21	30	30	0	0
4	D	14	20	20	1	0
5	B	37	0	20	0	0
5	C	37	0	20	0	0
6	A	174	0	0	2	1
6	B	144	0	0	5	1
6	C	167	0	0	6	0
6	D	167	0	0	1	0
All	All	7254	6907	6955	66	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 5.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:NH1	1:A:88:GLU:OE2	1.96	0.99
1:A:155:LYS:HE2	6:B:450:HOH:O	1.66	0.93
2:C:37:LYS:H	2:C:37:LYS:HE2	1.35	0.91
1:A:64:LYS:NZ	6:A:401:HOH:O	2.04	0.90
1:D:44:ASN:O	1:D:69:LYS:NZ	2.14	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:GLU:HG2	2:B:203:ALA:HB1	1.71	0.72
2:C:37:LYS:H	2:C:37:LYS:CE	2.01	0.71
1:D:155:LYS:HE2	6:C:459:HOH:O	1.95	0.65
2:B:44:GLN:CD	6:B:401:HOH:O	2.36	0.64
1:D:110:VAL:O	2:B:92:ARG:HD2	1.99	0.61
1:D:69:LYS:NZ	6:D:404:HOH:O	2.36	0.57
2:B:94:GLY:HA3	4:B:303:PEG:H12	1.87	0.57
4:A:303:PEG:O2	4:A:304:PEG:O4	2.17	0.54
2:C:150:PRO:HB2	2:C:202:GLU:HG3	1.90	0.53
2:B:94:GLY:CA	4:B:303:PEG:H12	2.39	0.53
2:C:108:GLU:HG3	2:C:154:LYS:HA	1.90	0.53
2:C:10:ARG:HG2	2:C:215:ALA:HB3	1.91	0.52
2:C:121:MET:HG2	2:C:123:PRO:HD3	1.91	0.52
2:B:6:LYS:HE2	2:B:215:ALA:HA	1.90	0.52
1:A:213:THR:O	4:A:303:PEG:C2	2.58	0.52
2:C:122:ILE:HG22	2:C:122:ILE:O	2.10	0.52
1:A:8:LYS:O	1:A:8:LYS:HG3	2.09	0.51
1:D:41:ASN:HD21	4:D:303:PEG:H41	1.76	0.51
1:A:84:ARG:O	1:A:88:GLU:HG3	2.11	0.51
2:B:94:GLY:O	2:B:136:LYS:HE2	2.11	0.51
2:C:17:LYS:HD2	2:C:40:HIS:H	1.75	0.49
1:D:55:GLU:OE2	1:D:80:PRO:HG2	2.13	0.48
2:B:44:GLN:NE2	6:B:401:HOH:O	2.46	0.48
2:B:108:GLU:HG3	2:B:154:LYS:HA	1.96	0.48
1:A:158:ASP:HA	1:A:191:VAL:O	2.14	0.48
2:C:177:GLU:HG3	6:C:443:HOH:O	2.14	0.47
2:B:177:GLU:HG3	6:B:424:HOH:O	2.14	0.47
1:D:84:ARG:NH1	1:D:88:GLU:OE1	2.47	0.47
1:A:172:PHE:O	1:A:176:MET:HG3	2.15	0.46
1:A:157:ALA:HA	1:A:162:ASN:O	2.15	0.46
2:C:10:ARG:HB2	2:C:215:ALA:CB	2.46	0.46
2:C:37:LYS:HE2	2:C:37:LYS:N	2.16	0.46
2:B:107:ASP:HA	2:B:153:VAL:O	2.16	0.46
2:C:108:GLU:HG2	2:C:203:ALA:HB1	1.98	0.46
1:D:54:PHE:O	1:D:60:GLY:HA3	2.16	0.46
4:A:303:PEG:O2	6:A:402:HOH:O	2.21	0.45
2:B:121:MET:HG3	2:B:123:PRO:HD3	1.98	0.44
2:C:25:ILE:HG12	6:C:486:HOH:O	2.18	0.44
2:C:40:HIS:HB3	6:C:532:HOH:O	2.17	0.44
2:B:10:ARG:HB2	2:B:215:ALA:HB3	2.01	0.43
2:C:6:LYS:CE	2:C:215:ALA:HA	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:44[B]:GLN:HG2	2:C:49:ILE:O	2.18	0.43
2:B:10:ARG:HB2	2:B:215:ALA:CB	2.48	0.42
2:C:165:LYS:HD3	6:C:531:HOH:O	2.19	0.42
2:B:6:LYS:CE	2:B:215:ALA:HA	2.49	0.42
1:D:16:GLY:HA2	1:D:44:ASN:O	2.19	0.42
2:C:10:ARG:CG	2:C:215:ALA:HB3	2.50	0.42
2:B:10:ARG:HG2	2:B:215:ALA:HB3	2.01	0.42
2:B:44:GLN:CG	6:B:401:HOH:O	2.67	0.42
1:D:49:ALA:O	1:D:73:VAL:HA	2.19	0.41
2:C:38:ASP:OD1	2:C:38:ASP:N	2.39	0.41
1:D:46:THR:OG1	1:D:69:LYS:HE2	2.20	0.41
2:C:165:LYS:CD	6:C:531:HOH:O	2.68	0.41
1:D:50:ASN:OD1	1:D:98:GLN:HG3	2.21	0.41
1:D:158:ASP:HA	1:D:191:VAL:O	2.20	0.41
2:C:5:GLU:O	2:C:9:ILE:HG13	2.21	0.41
1:A:49:ALA:O	1:A:73:VAL:HA	2.21	0.40
1:A:155:LYS:HA	1:A:155:LYS:HD3	1.83	0.40
1:A:213:THR:O	4:A:303:PEG:C1	2.70	0.40
1:A:206:ILE:HG12	2:C:20:LEU:HB2	2.03	0.40
2:B:184:LEU:HD23	2:B:186:LYS:HD3	2.04	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:A:402:HOH:O	6:B:462:HOH:O[7_555]	2.06	0.14

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	214/217 (99%)	211 (99%)	2 (1%)	1 (0%)	25 17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	212/217 (98%)	208 (98%)	3 (1%)	1 (0%)	25 17
2	B	212/215 (99%)	207 (98%)	4 (2%)	1 (0%)	25 17
2	C	213/215 (99%)	207 (97%)	5 (2%)	1 (0%)	25 17
All	All	851/864 (98%)	833 (98%)	14 (2%)	4 (0%)	25 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	214	PHE
2	B	214	PHE
1	D	171	ASN
1	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	A	181/181 (100%)	179 (99%)	2 (1%)	70 71
1	D	179/181 (99%)	175 (98%)	4 (2%)	47 43
2	B	173/175 (99%)	170 (98%)	3 (2%)	56 54
2	C	174/175 (99%)	169 (97%)	5 (3%)	37 31
All	All	707/712 (99%)	693 (98%)	14 (2%)	50 47

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	29	THR
1	D	39	ARG
1	D	115	ILE
1	D	155	LYS
1	A	115	ILE
1	A	181	LYS
2	C	17	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	37	LYS
2	C	125	MET
2	C	164	ARG
2	C	204	LYS
2	B	2	ASN
2	B	125	MET
2	B	164	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

17 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	$\#\|Z\| > 2$
3	ACT	D	301	-	3,3,3	1.01	0	3,3,3	1.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PEG	B	303	-	6,6,6	0.29	0	5,5,5	0.25	0
4	PEG	D	303	-	6,6,6	0.28	0	5,5,5	0.27	0
4	PEG	A	302	-	6,6,6	0.21	0	5,5,5	0.27	0
3	ACT	B	301	-	3,3,3	1.54	1 (33%)	3,3,3	1.07	0
5	COA	C	305	-	35,39,50	2.94	14 (40%)	44,61,75	1.61	9 (20%)
3	ACT	A	301	-	3,3,3	1.09	0	3,3,3	1.41	0
3	ACT	C	302	-	3,3,3	1.32	0	3,3,3	1.26	0
4	PEG	B	302	-	6,6,6	0.45	0	5,5,5	0.63	0
4	PEG	C	304	-	6,6,6	0.42	0	5,5,5	0.36	0
4	PEG	D	302	-	6,6,6	0.26	0	5,5,5	0.28	0
4	PEG	A	304	-	6,6,6	0.44	0	5,5,5	0.25	0
4	PEG	C	303	-	6,6,6	0.22	0	5,5,5	0.22	0
5	COA	B	304	-	35,39,50	2.87	15 (42%)	44,61,75	1.60	10 (22%)
4	PEG	A	303	-	3,3,6	0.34	0	2,2,5	0.32	0
4	PEG	A	305	-	6,6,6	0.22	0	5,5,5	0.16	0
4	PEG	C	301	-	6,6,6	0.22	0	5,5,5	0.14	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	PEG	B	303	-	-	1/4/4/4	-
4	PEG	A	302	-	-	1/4/4/4	-
4	PEG	D	303	-	-	2/4/4/4	-
5	COA	C	305	-	-	8/27/47/64	0/3/3/3
4	PEG	B	302	-	-	1/4/4/4	-
4	PEG	C	304	-	-	1/4/4/4	-
4	PEG	D	302	-	-	1/4/4/4	-
4	PEG	A	304	-	-	0/4/4/4	-
4	PEG	C	303	-	-	1/4/4/4	-
5	COA	B	304	-	-	7/27/47/64	0/3/3/3
4	PEG	A	303	-	-	1/1/1/4	-
4	PEG	A	305	-	-	1/4/4/4	-
4	PEG	C	301	-	-	2/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	305	COA	O4B-C1B	10.15	1.54	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	304	COA	O4B-C1B	9.73	1.53	1.40
5	C	305	COA	P1A-O3A	6.03	1.66	1.59
5	C	305	COA	P2A-O3A	5.76	1.65	1.59
5	B	304	COA	P1A-O3A	5.46	1.65	1.59
5	B	304	COA	P2A-O3A	5.02	1.64	1.59
5	B	304	COA	C1B-N9A	-4.71	1.38	1.49
5	C	305	COA	C1B-N9A	-4.62	1.38	1.49
5	B	304	COA	C5A-N7A	4.30	1.55	1.39
5	C	305	COA	C5A-N7A	3.97	1.54	1.39
5	B	304	COA	O4B-C4B	3.68	1.53	1.45
5	C	305	COA	O4B-C4B	3.59	1.53	1.45
5	C	305	COA	C4A-N3A	-3.27	1.31	1.35
5	C	305	COA	C2B-C3B	-2.96	1.46	1.53
5	B	304	COA	O2B-C2B	2.92	1.50	1.43
5	B	304	COA	C4A-N3A	-2.86	1.31	1.35
5	B	304	COA	C2B-C3B	-2.81	1.46	1.53
5	B	304	COA	C6A-N6A	2.68	1.43	1.34
5	B	304	COA	P3B-O3B	2.57	1.64	1.59
5	C	305	COA	C6A-N6A	2.56	1.43	1.34
5	B	304	COA	C2A-N3A	2.56	1.36	1.32
5	C	305	COA	O2B-C2B	2.52	1.49	1.43
5	B	304	COA	P3B-O8A	-2.38	1.46	1.54
5	B	304	COA	P3B-O9A	-2.30	1.46	1.54
3	B	301	ACT	CH3-C	2.27	1.58	1.49
5	C	305	COA	P3B-O3B	2.24	1.63	1.59
5	C	305	COA	P3B-O8A	-2.16	1.46	1.54
5	C	305	COA	C2A-N3A	2.12	1.35	1.32
5	C	305	COA	P3B-O9A	-2.07	1.47	1.54
5	B	304	COA	P1A-O2A	-2.01	1.46	1.55

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	305	COA	C4B-O4B-C1B	-5.21	105.16	109.92
5	B	304	COA	C4B-O4B-C1B	-4.69	105.63	109.92
5	C	305	COA	N3A-C2A-N1A	-3.18	124.36	128.67
5	C	305	COA	P3B-O3B-C3B	-3.17	114.97	123.43
5	C	305	COA	C4A-C5A-N7A	-3.03	106.13	109.34
5	B	304	COA	C3B-C2B-C1B	2.81	106.08	99.89
5	B	304	COA	O5A-P2A-O3A	2.73	114.65	107.27
5	C	305	COA	O4B-C1B-N9A	2.70	112.33	108.75
5	C	305	COA	O3B-C3B-C2B	-2.69	102.04	111.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	304	COA	O3B-C3B-C2B	-2.67	102.11	111.68
5	B	304	COA	N3A-C2A-N1A	-2.67	125.05	128.67
5	B	304	COA	C4A-C5A-N7A	-2.54	106.66	109.34
5	C	305	COA	C3B-C2B-C1B	2.52	105.43	99.89
5	B	304	COA	C1B-N9A-C4A	-2.47	122.30	126.64
5	C	305	COA	C1B-N9A-C4A	-2.32	122.56	126.64
5	B	304	COA	P3B-O3B-C3B	-2.26	117.39	123.43
5	C	305	COA	N6A-C6A-N1A	2.14	122.91	118.33
5	B	304	COA	C2B-C3B-C4B	2.11	106.93	103.24
5	B	304	COA	N6A-C6A-N1A	2.08	122.78	118.33

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	305	COA	P2A-O3A-P1A-O5B
5	C	305	COA	P1A-O3A-P2A-O6A
5	C	305	COA	OAP-CAP-CBP-CCP
5	C	305	COA	OAP-CAP-CBP-CDP
5	C	305	COA	OAP-CAP-CBP-CEP
5	B	304	COA	P2A-O3A-P1A-O5B
5	B	304	COA	P1A-O3A-P2A-O6A
5	B	304	COA	OAP-CAP-CBP-CCP
4	D	303	PEG	C4-C3-O2-C2
4	A	302	PEG	O2-C3-C4-O4
4	C	301	PEG	O2-C3-C4-O4
4	C	303	PEG	O2-C3-C4-O4
4	C	304	PEG	O2-C3-C4-O4
4	B	303	PEG	O2-C3-C4-O4
4	D	303	PEG	O1-C1-C2-O2
4	A	305	PEG	O2-C3-C4-O4
4	A	303	PEG	O1-C1-C2-O2
4	B	302	PEG	O1-C1-C2-O2
4	D	302	PEG	O2-C3-C4-O4
4	C	301	PEG	O1-C1-C2-O2
5	C	305	COA	C5B-O5B-P1A-O1A
5	C	305	COA	C5B-O5B-P1A-O2A
5	C	305	COA	C5B-O5B-P1A-O3A
5	B	304	COA	C5B-O5B-P1A-O2A
5	B	304	COA	C5B-O5B-P1A-O3A
5	B	304	COA	OAP-CAP-CBP-CDP
5	B	304	COA	OAP-CAP-CBP-CEP

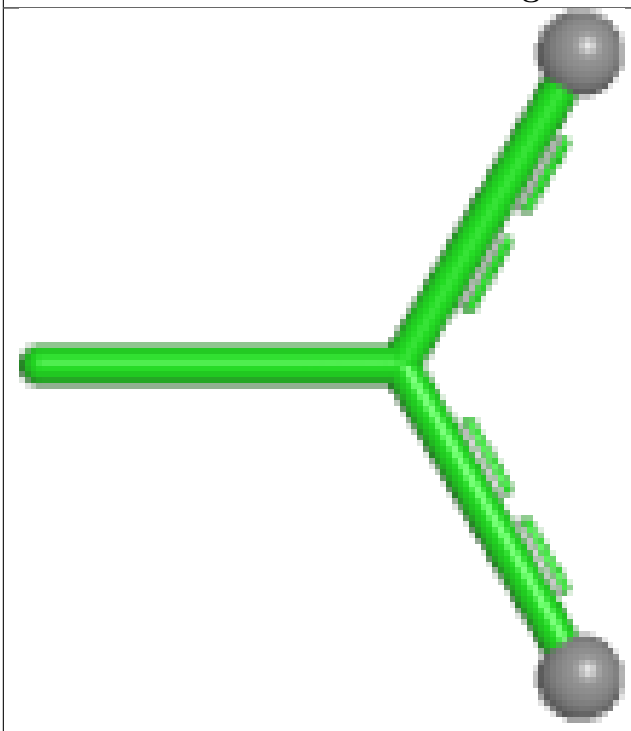
There are no ring outliers.

4 monomers are involved in 7 short contacts:

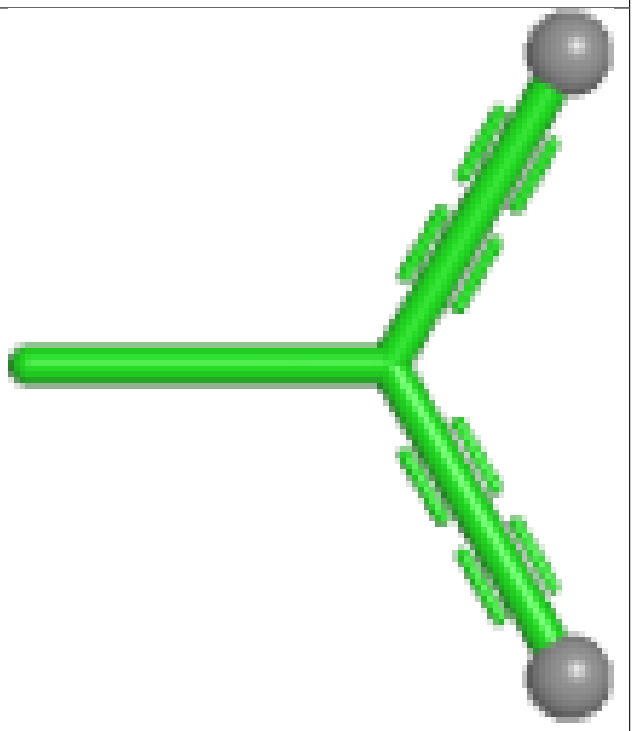
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	PEG	2	0
4	D	303	PEG	1	0
4	A	304	PEG	1	0
4	A	303	PEG	4	0

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.

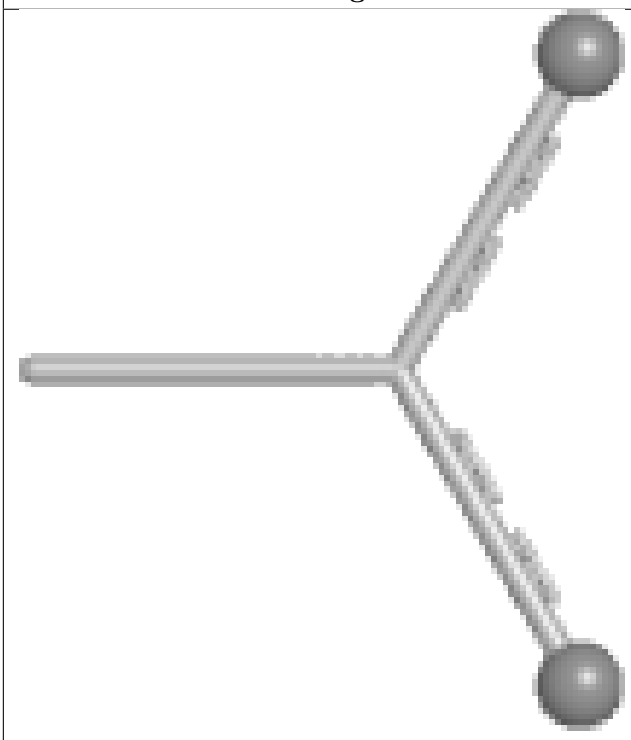
Ligand ACT D 301



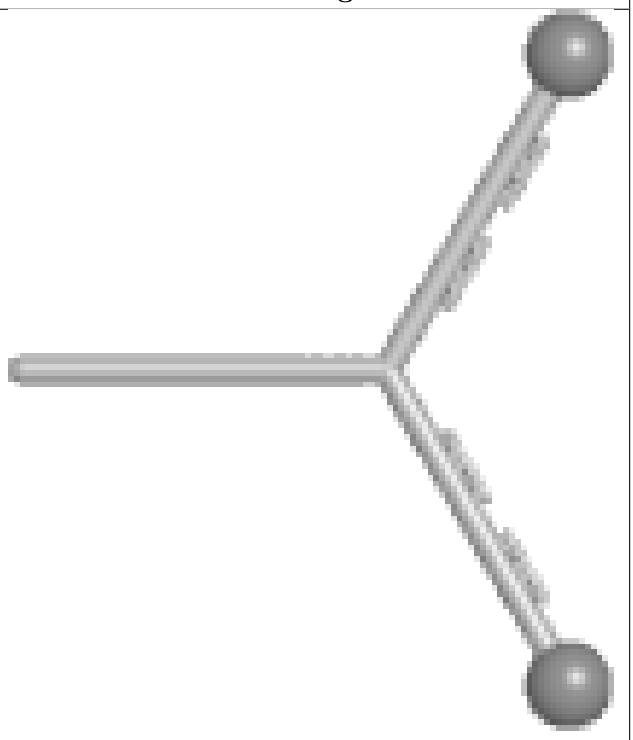
Bond lengths



Bond angles

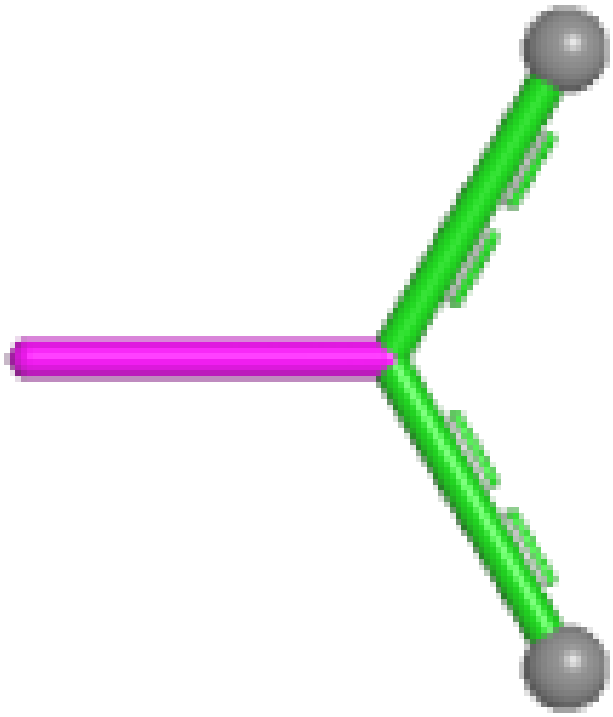


Torsions

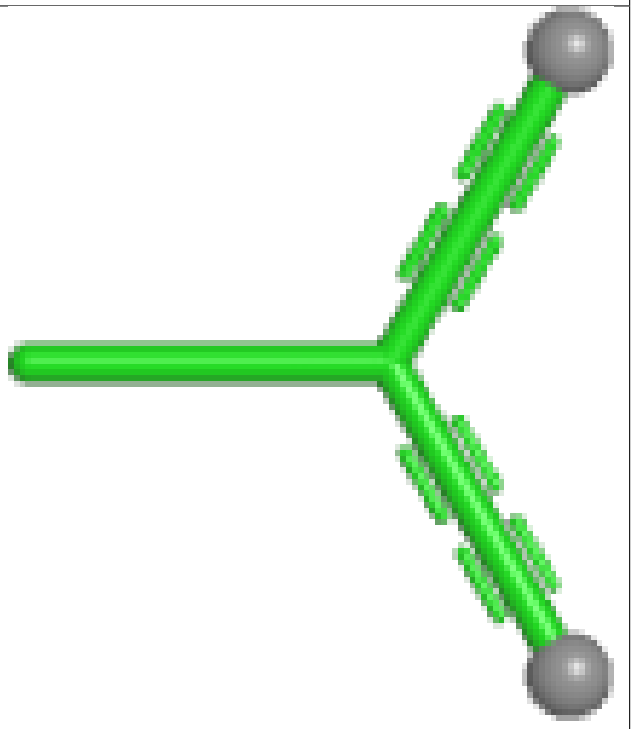


Rings

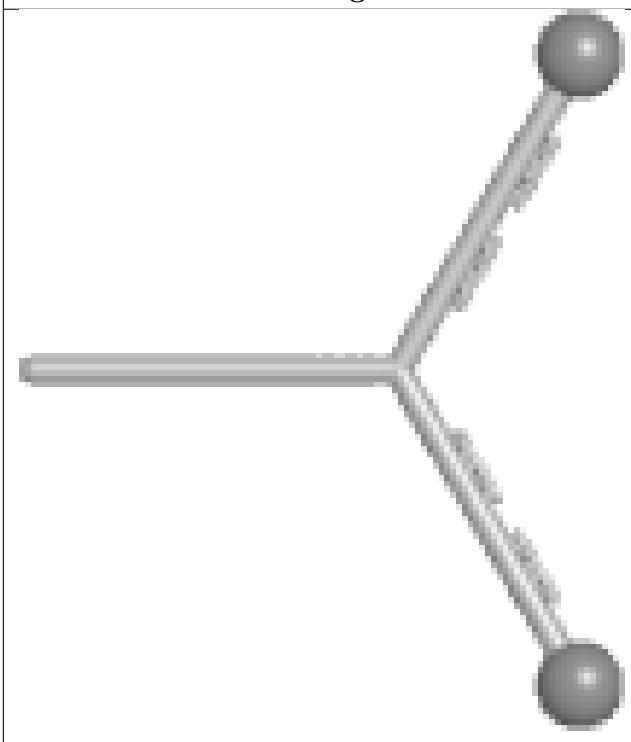
Ligand ACT B 301



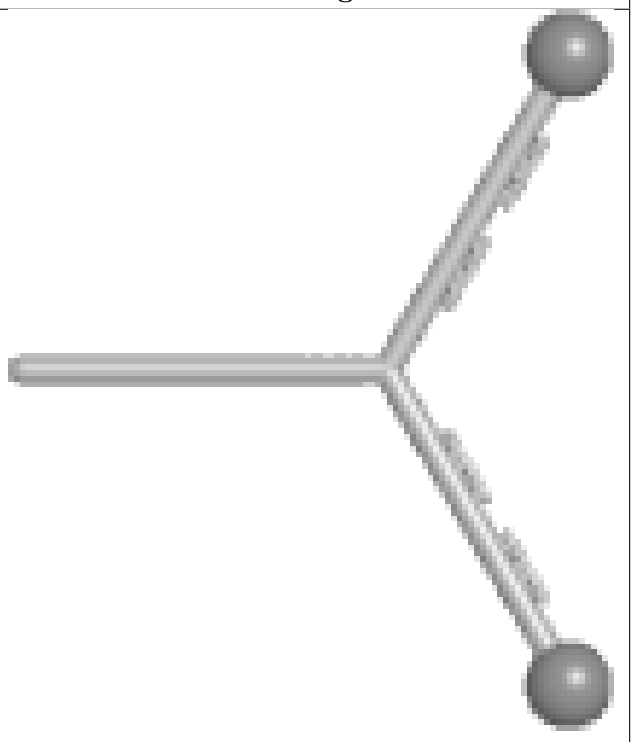
Bond lengths



Bond angles

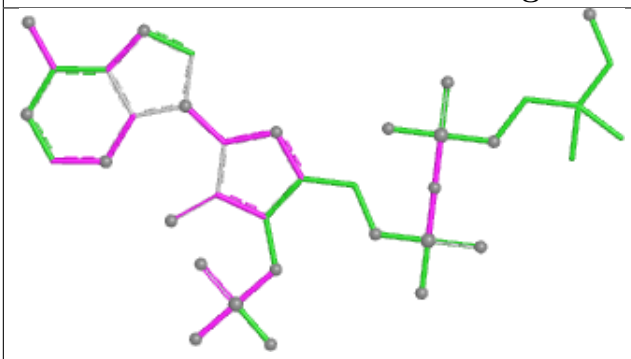


Torsions

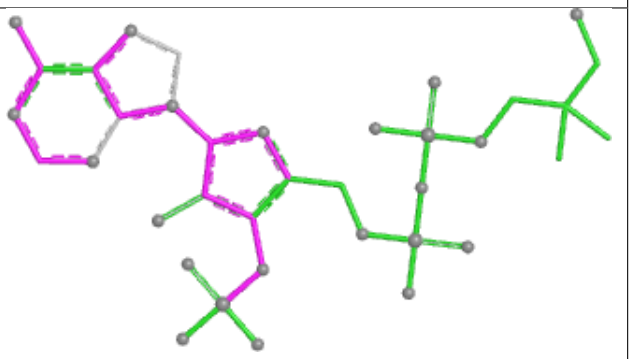


Rings

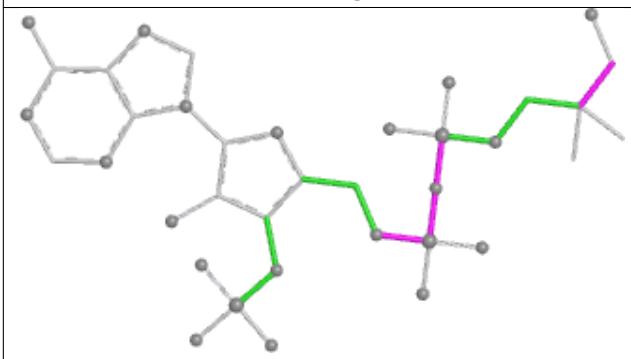
Ligand COA C 305



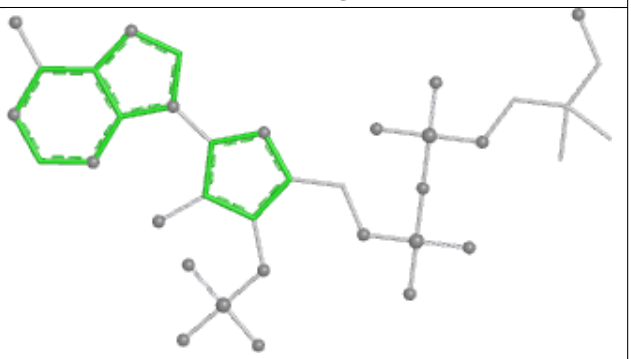
Bond lengths



Bond angles

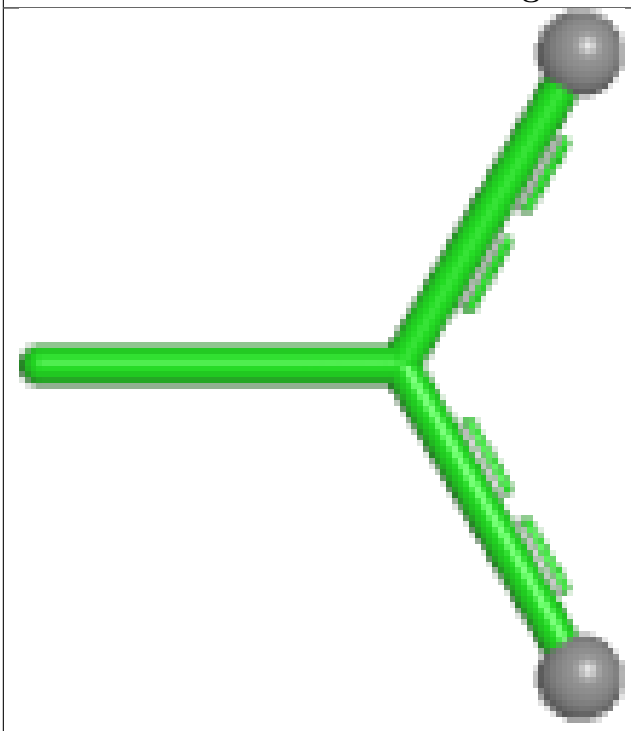


Torsions

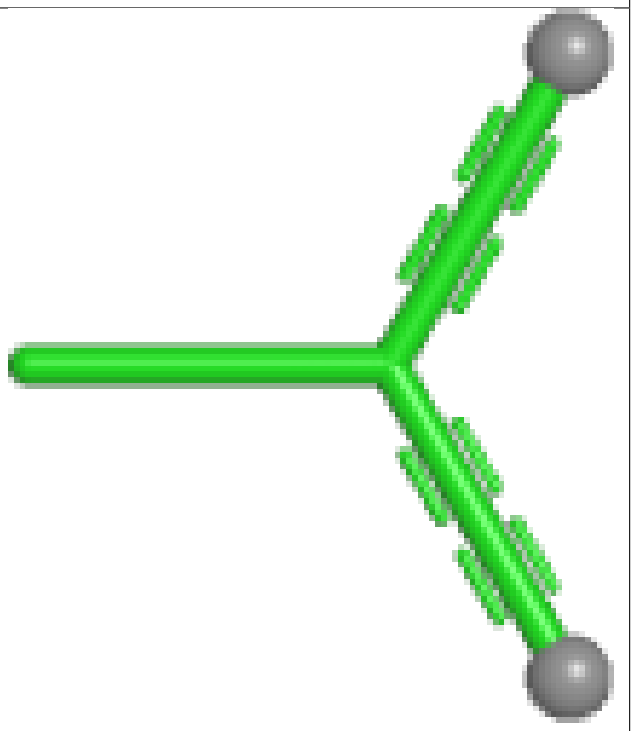


Rings

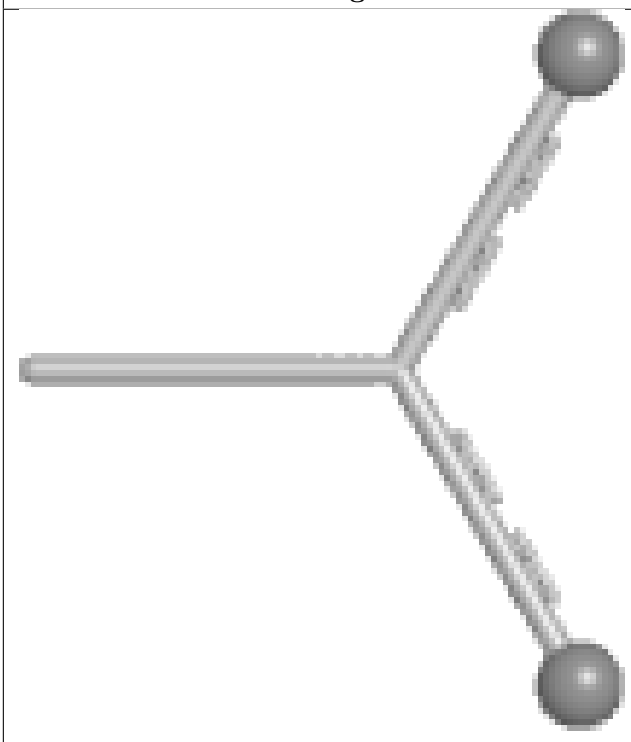
Ligand ACT A 301



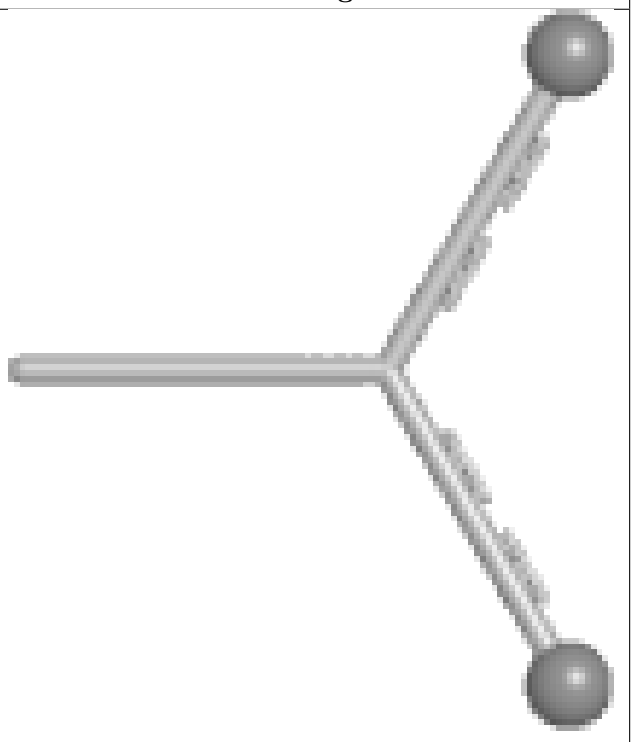
Bond lengths



Bond angles

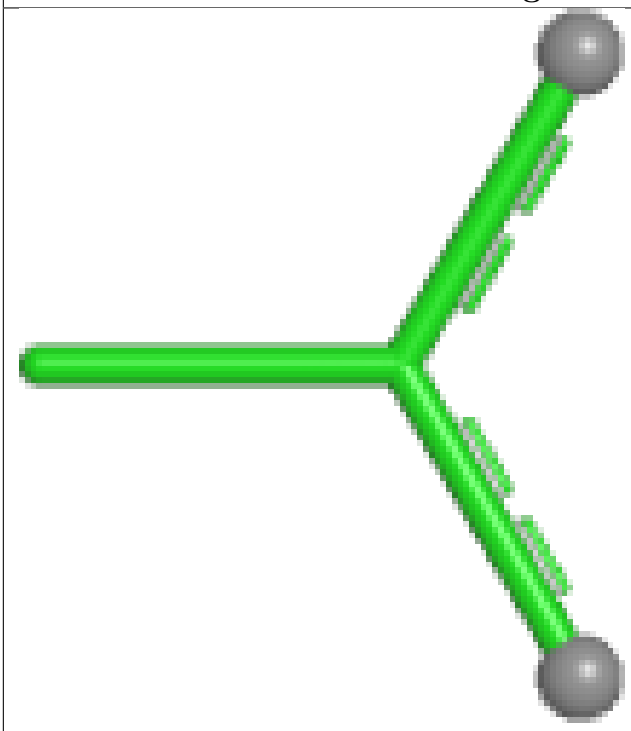


Torsions

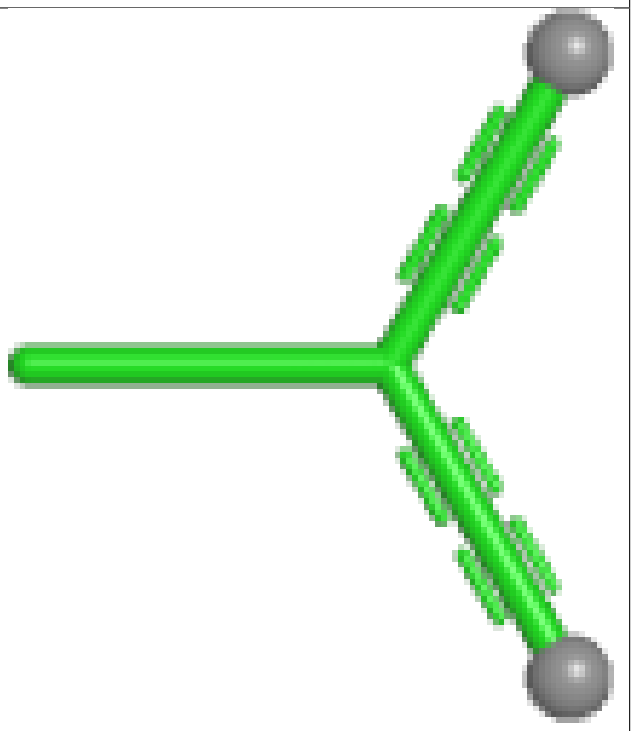


Rings

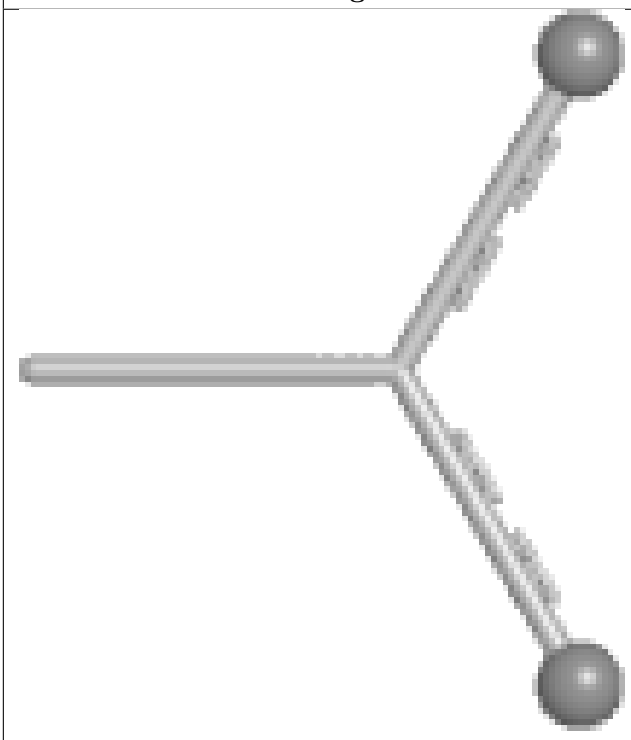
Ligand ACT C 302



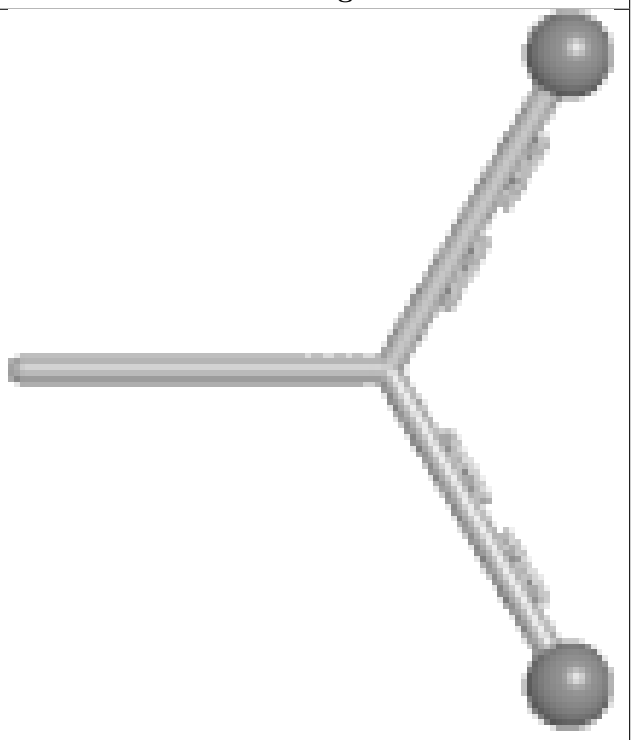
Bond lengths



Bond angles

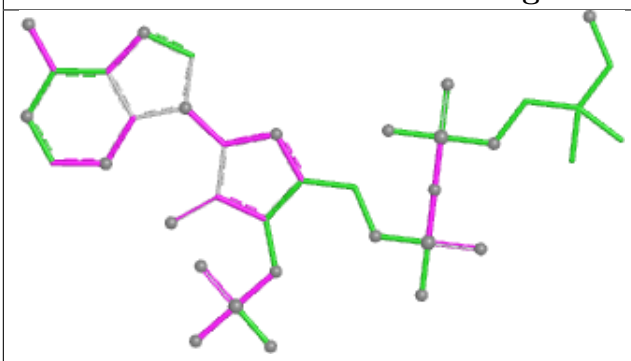


Torsions

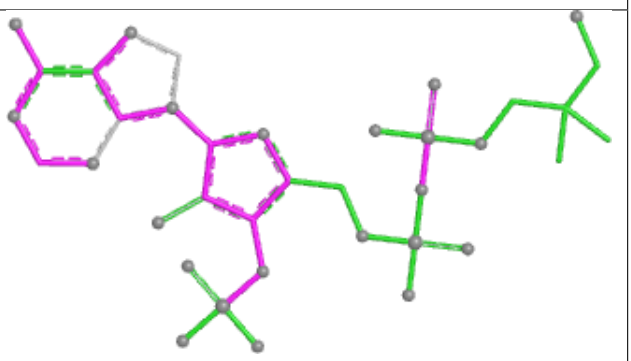


Rings

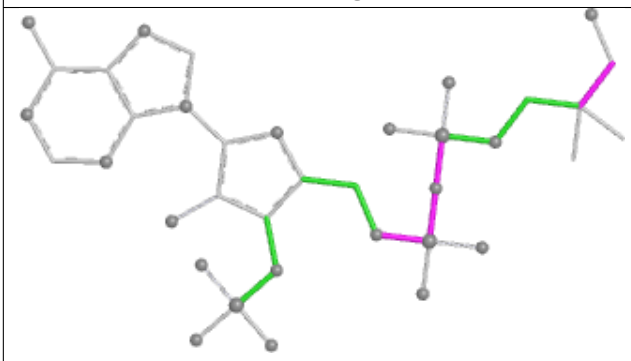
Ligand COA B 304



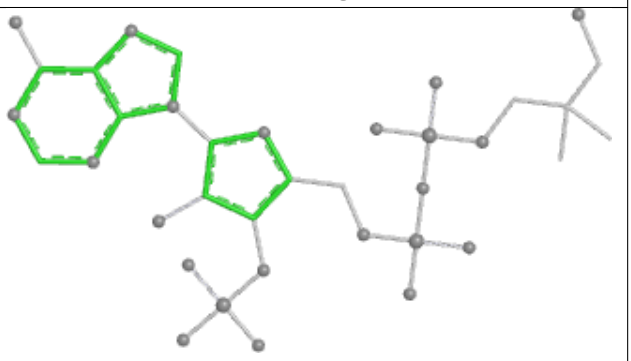
Bond lengths



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	213/217 (98%)	-0.93	2 (0%)	81	82	6, 16, 40, 55	3 (1%)
1	D	213/217 (98%)	-0.87	3 (1%)	73	75	6, 17, 42, 59	1 (0%)
2	B	214/215 (99%)	-0.42	8 (3%)	45	47	11, 23, 49, 73	0
2	C	214/215 (99%)	-0.44	8 (3%)	45	47	8, 23, 48, 66	1 (0%)
All	All	854/864 (98%)	-0.66	21 (2%)	58	60	6, 19, 46, 73	5 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	PHE	7.0
2	B	215	ALA	5.8
2	C	214	PHE	5.8
1	A	213	THR	5.6
2	C	215	ALA	4.8
2	B	210	ASP	3.0
1	D	69	LYS	2.6
1	D	213	THR	2.6
2	C	122	ILE	2.4
1	D	136	GLY	2.4
2	B	2	ASN	2.3
2	C	2	ASN	2.3
2	C	25	ILE	2.3
2	C	209	ASP	2.2
2	C	37	LYS	2.2
2	B	121	MET	2.1
2	B	122	ILE	2.1
2	C	120	LYS	2.1
2	B	37	LYS	2.1
2	B	120	LYS	2.0
1	A	1	MET	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)

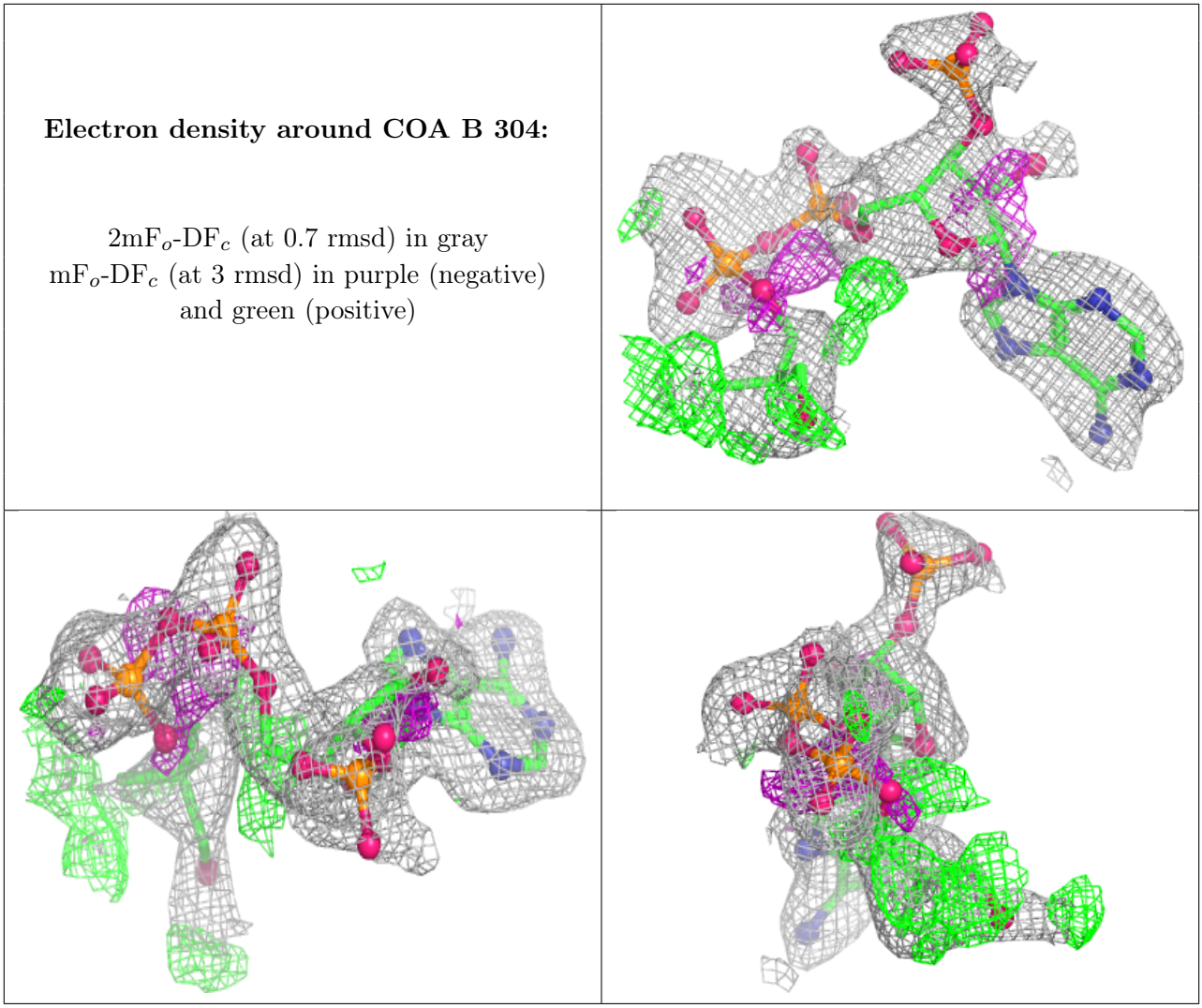
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	PEG	D	303	7/7	0.61	0.25	42,56,70,72	0
4	PEG	C	301	7/7	0.69	0.20	45,55,72,80	0
4	PEG	B	303	7/7	0.70	0.23	33,40,65,71	0
4	PEG	C	304	7/7	0.71	0.24	35,45,61,73	0
5	COA	B	304	37/48	0.72	0.18	33,54,90,113	0
4	PEG	A	303	4/7	0.73	0.23	30,36,42,52	0
4	PEG	A	304	7/7	0.74	0.21	30,43,61,74	0
4	PEG	A	305	7/7	0.75	0.23	44,55,80,80	0
4	PEG	C	303	7/7	0.78	0.17	37,46,59,70	0
4	PEG	D	302	7/7	0.79	0.18	30,51,78,93	0
5	COA	C	305	37/48	0.80	0.15	27,46,68,100	0
4	PEG	B	302	7/7	0.81	0.22	23,32,62,74	0
4	PEG	A	302	7/7	0.84	0.15	32,45,54,59	0
3	ACT	B	301	4/4	0.95	0.07	18,19,21,21	0
3	ACT	C	302	4/4	0.96	0.09	18,21,22,28	0
3	ACT	D	301	4/4	0.97	0.05	13,15,17,20	0
3	ACT	A	301	4/4	0.98	0.05	15,15,18,19	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.

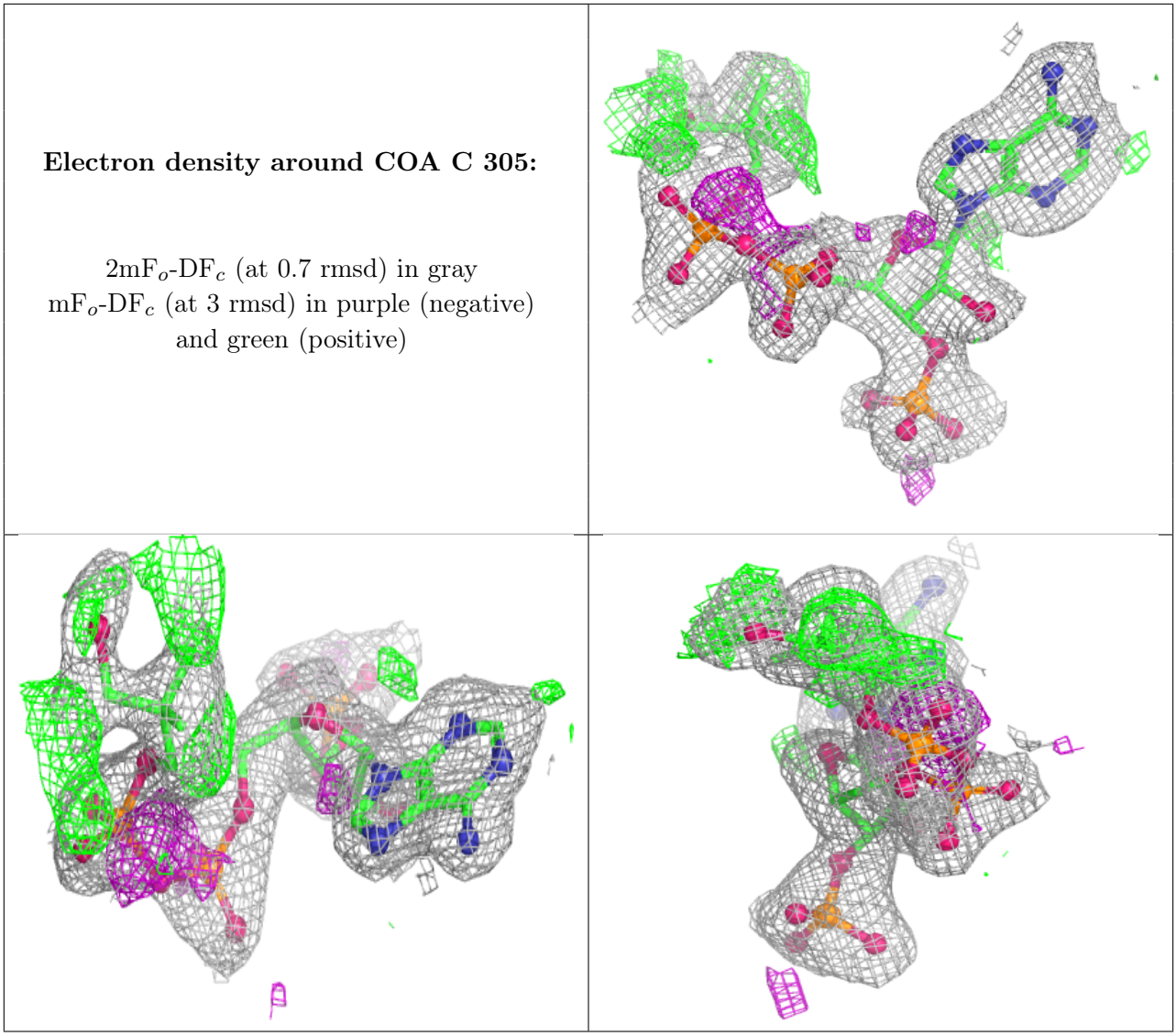
Electron density around COA B 304:

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



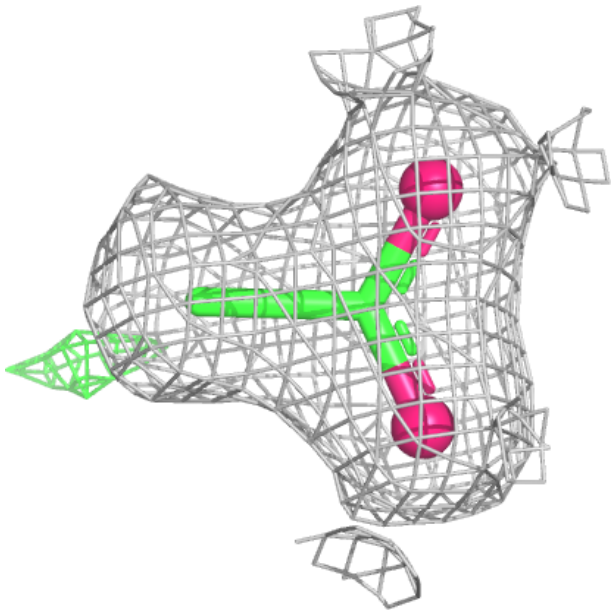
Electron density around COA C 305:

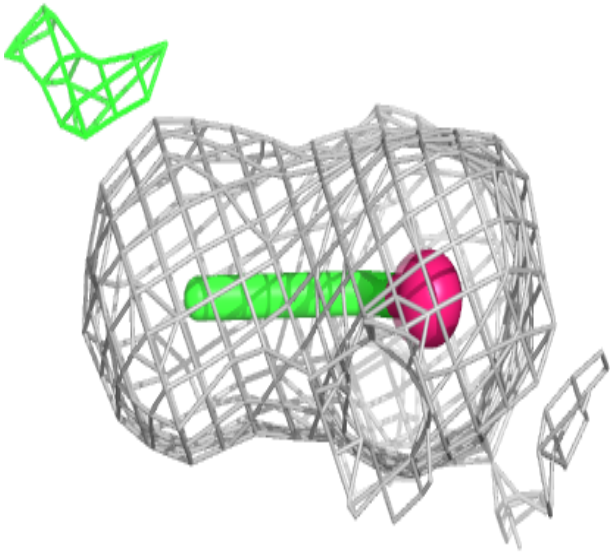
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

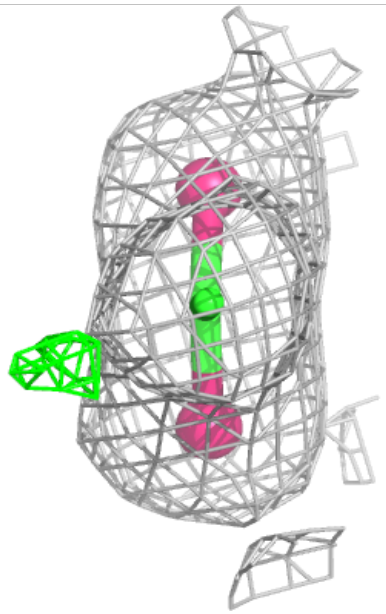


Electron density around ACT B 301:

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

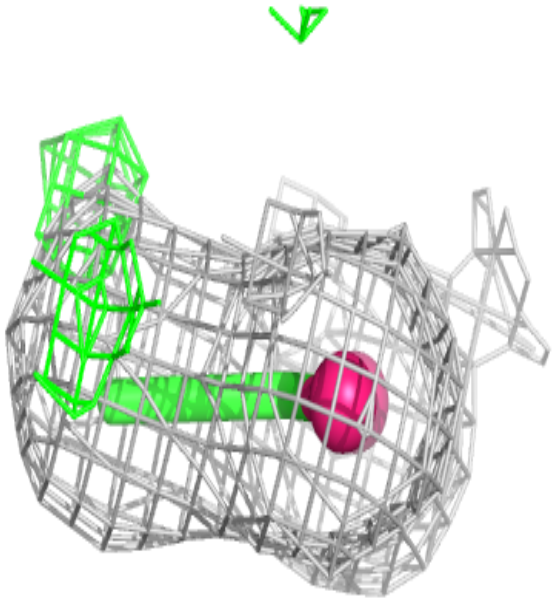


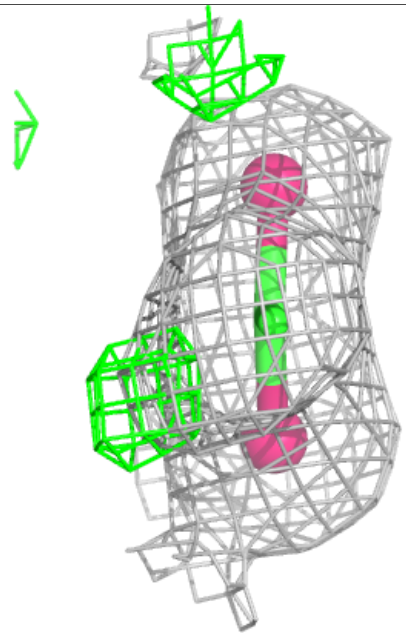




Electron density around ACT C 302:

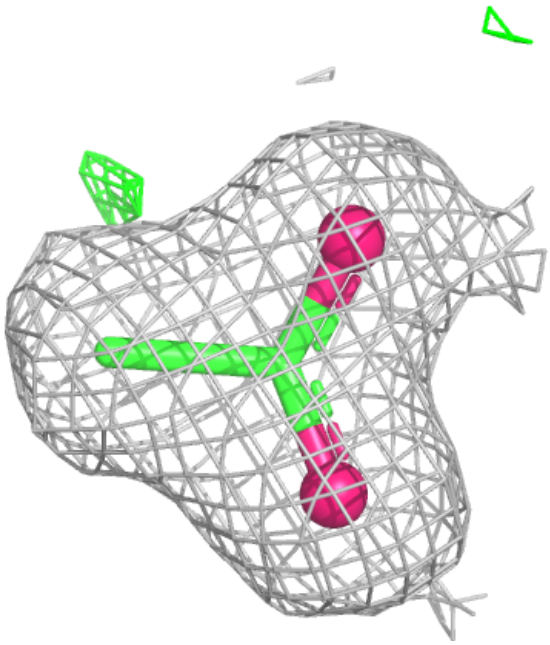
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

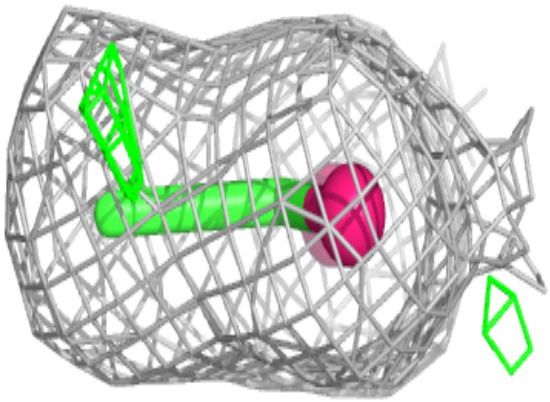


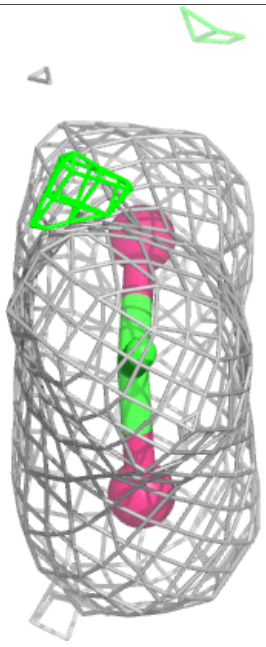


Electron density around ACT D 301:

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

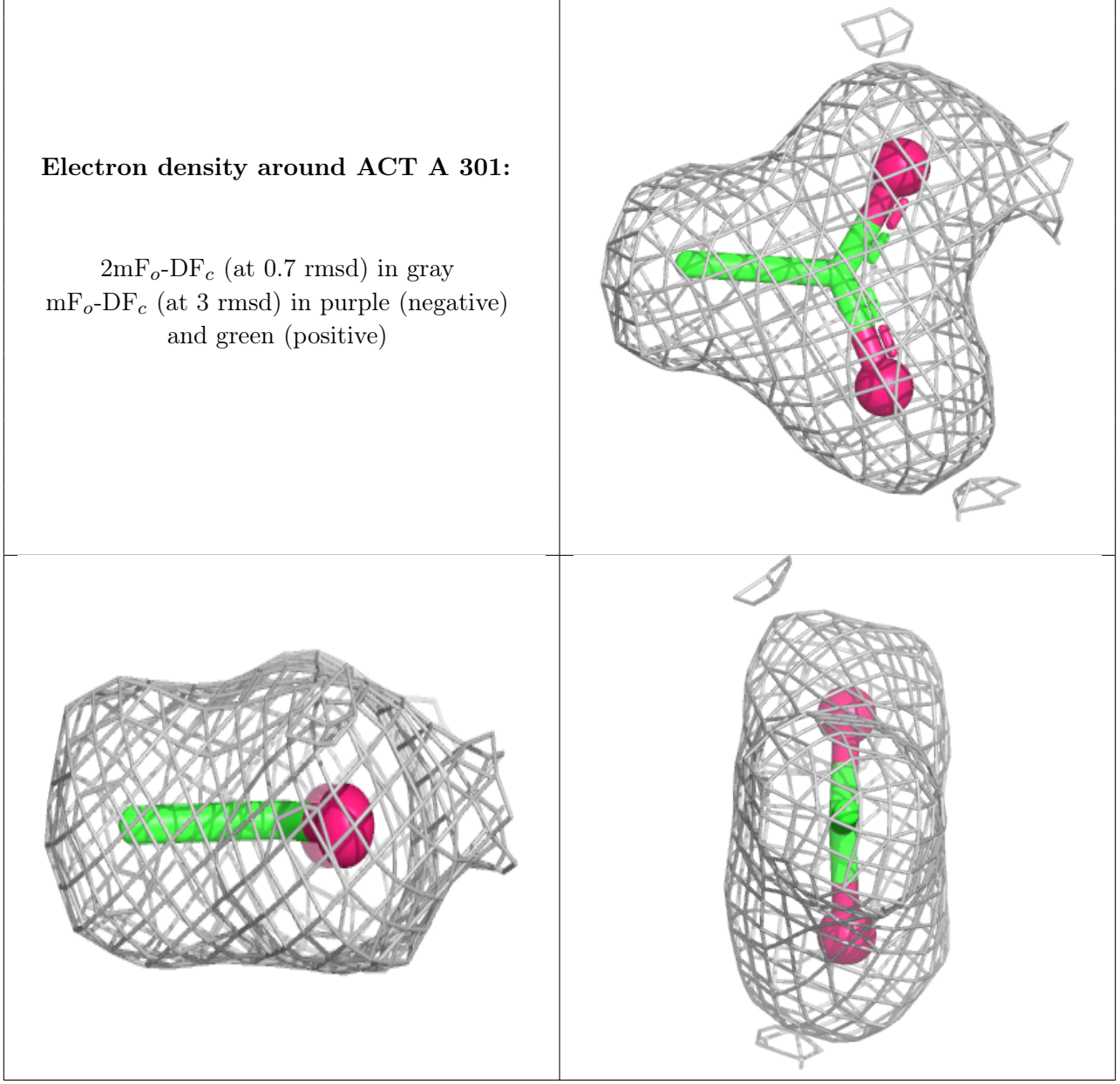






Electron density around ACT A 301:

$2mF_o$-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.