



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2022 – 10:10 AM EDT

PDB ID : 7SKJ
Title : Crystal structure of chloroplast triosephosphate isomerase from *Cuscuta australis*
Authors : Jones, G.; Vickers, C.; Patrick, W.
Deposited on : 2021-10-20
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

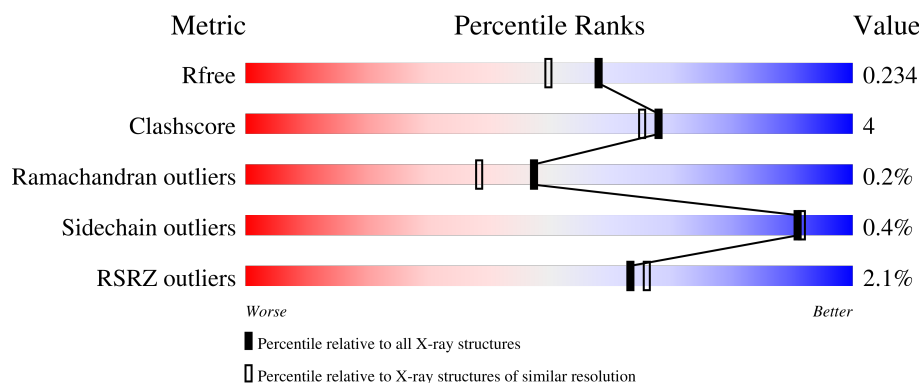
1 Overall quality at a glance

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 $\leq 5\%$. 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	275	<div> <div>3%</div> <div>84%</div> <div>5%</div> <div>11%</div> </div>
1	B	275	<div> <div>80%</div> <div>8%</div> <div>12%</div> </div>
1	C	275	<div> <div>%</div> <div>83%</div> <div>5%</div> <div>12%</div> </div>
1	D	275	<div> <div>4%</div> <div>75%</div> <div>11%</div> <div>14%</div> </div>

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
2	ACT	A	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7966 atoms, of which 3 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 Triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1823	1154	316	345	8			
1	B	243	Total	C	N	O	S	0	0	0
			1790	1133	309	340	8			
1	C	242	Total	C	N	O	S	0	0	0
			1758	1114	299	337	8			
1	D	237	Total	C	N	O	S	0	0	0
			1692	1069	291	324	8			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A0A328DYS8
A	-17	GLY	-	expression tag	UNP A0A328DYS8
A	-16	SER	-	expression tag	UNP A0A328DYS8
A	-15	SER	-	expression tag	UNP A0A328DYS8
A	-14	HIS	-	expression tag	UNP A0A328DYS8
A	-13	HIS	-	expression tag	UNP A0A328DYS8
A	-12	HIS	-	expression tag	UNP A0A328DYS8
A	-11	HIS	-	expression tag	UNP A0A328DYS8
A	-10	HIS	-	expression tag	UNP A0A328DYS8
A	-9	HIS	-	expression tag	UNP A0A328DYS8
A	-8	SER	-	expression tag	UNP A0A328DYS8
A	-7	SER	-	expression tag	UNP A0A328DYS8
A	-6	GLY	-	expression tag	UNP A0A328DYS8
A	-5	LEU	-	expression tag	UNP A0A328DYS8
A	-4	VAL	-	expression tag	UNP A0A328DYS8
A	-3	PRO	-	expression tag	UNP A0A328DYS8
A	-2	ARG	-	expression tag	UNP A0A328DYS8
A	-1	GLY	-	expression tag	UNP A0A328DYS8
A	0	SER	-	expression tag	UNP A0A328DYS8
A	1	HIS	-	expression tag	UNP A0A328DYS8
B	-18	MET	-	initiating methionine	UNP A0A328DYS8

Continued on next page...

Continued from previous page...

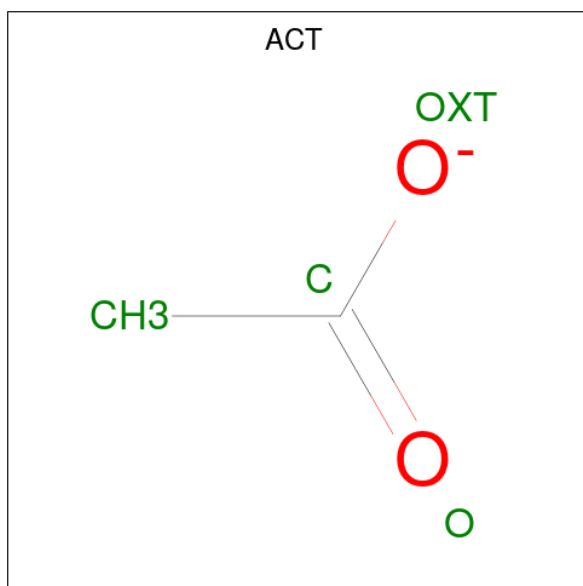
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	GLY	-	expression tag	UNP A0A328DYS8
B	-16	SER	-	expression tag	UNP A0A328DYS8
B	-15	SER	-	expression tag	UNP A0A328DYS8
B	-14	HIS	-	expression tag	UNP A0A328DYS8
B	-13	HIS	-	expression tag	UNP A0A328DYS8
B	-12	HIS	-	expression tag	UNP A0A328DYS8
B	-11	HIS	-	expression tag	UNP A0A328DYS8
B	-10	HIS	-	expression tag	UNP A0A328DYS8
B	-9	HIS	-	expression tag	UNP A0A328DYS8
B	-8	SER	-	expression tag	UNP A0A328DYS8
B	-7	SER	-	expression tag	UNP A0A328DYS8
B	-6	GLY	-	expression tag	UNP A0A328DYS8
B	-5	LEU	-	expression tag	UNP A0A328DYS8
B	-4	VAL	-	expression tag	UNP A0A328DYS8
B	-3	PRO	-	expression tag	UNP A0A328DYS8
B	-2	ARG	-	expression tag	UNP A0A328DYS8
B	-1	GLY	-	expression tag	UNP A0A328DYS8
B	0	SER	-	expression tag	UNP A0A328DYS8
B	1	HIS	-	expression tag	UNP A0A328DYS8
C	-18	MET	-	initiating methionine	UNP A0A328DYS8
C	-17	GLY	-	expression tag	UNP A0A328DYS8
C	-16	SER	-	expression tag	UNP A0A328DYS8
C	-15	SER	-	expression tag	UNP A0A328DYS8
C	-14	HIS	-	expression tag	UNP A0A328DYS8
C	-13	HIS	-	expression tag	UNP A0A328DYS8
C	-12	HIS	-	expression tag	UNP A0A328DYS8
C	-11	HIS	-	expression tag	UNP A0A328DYS8
C	-10	HIS	-	expression tag	UNP A0A328DYS8
C	-9	HIS	-	expression tag	UNP A0A328DYS8
C	-8	SER	-	expression tag	UNP A0A328DYS8
C	-7	SER	-	expression tag	UNP A0A328DYS8
C	-6	GLY	-	expression tag	UNP A0A328DYS8
C	-5	LEU	-	expression tag	UNP A0A328DYS8
C	-4	VAL	-	expression tag	UNP A0A328DYS8
C	-3	PRO	-	expression tag	UNP A0A328DYS8
C	-2	ARG	-	expression tag	UNP A0A328DYS8
C	-1	GLY	-	expression tag	UNP A0A328DYS8
C	0	SER	-	expression tag	UNP A0A328DYS8
C	1	HIS	-	expression tag	UNP A0A328DYS8
D	-18	MET	-	initiating methionine	UNP A0A328DYS8
D	-17	GLY	-	expression tag	UNP A0A328DYS8
D	-16	SER	-	expression tag	UNP A0A328DYS8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	expression tag	UNP A0A328DYS8
D	-14	HIS	-	expression tag	UNP A0A328DYS8
D	-13	HIS	-	expression tag	UNP A0A328DYS8
D	-12	HIS	-	expression tag	UNP A0A328DYS8
D	-11	HIS	-	expression tag	UNP A0A328DYS8
D	-10	HIS	-	expression tag	UNP A0A328DYS8
D	-9	HIS	-	expression tag	UNP A0A328DYS8
D	-8	SER	-	expression tag	UNP A0A328DYS8
D	-7	SER	-	expression tag	UNP A0A328DYS8
D	-6	GLY	-	expression tag	UNP A0A328DYS8
D	-5	LEU	-	expression tag	UNP A0A328DYS8
D	-4	VAL	-	expression tag	UNP A0A328DYS8
D	-3	PRO	-	expression tag	UNP A0A328DYS8
D	-2	ARG	-	expression tag	UNP A0A328DYS8
D	-1	GLY	-	expression tag	UNP A0A328DYS8
D	0	SER	-	expression tag	UNP A0A328DYS8
D	1	HIS	-	expression tag	UNP A0A328DYS8

- Molecule 2 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
2	A	1	Total	C	O		0	0
			4	2	2			
2	C	1	Total	C	H	O	0	0
			7	2	3	2		

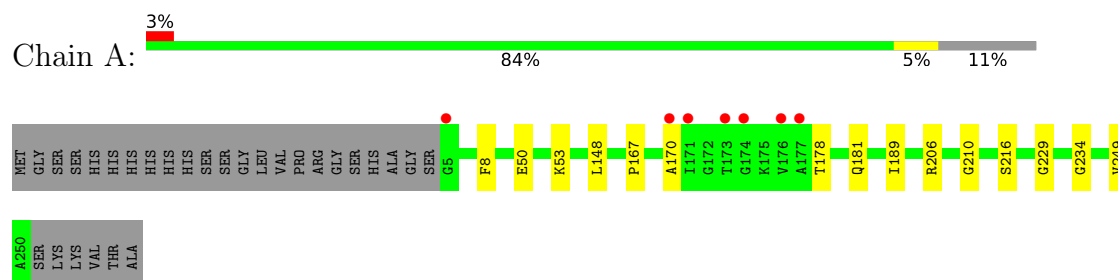
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	283	Total 283	O 283	0	0
3	B	273	Total 273	O 273	0	0
3	C	186	Total 186	O 186	0	0
3	D	150	Total 150	O 150	0	0

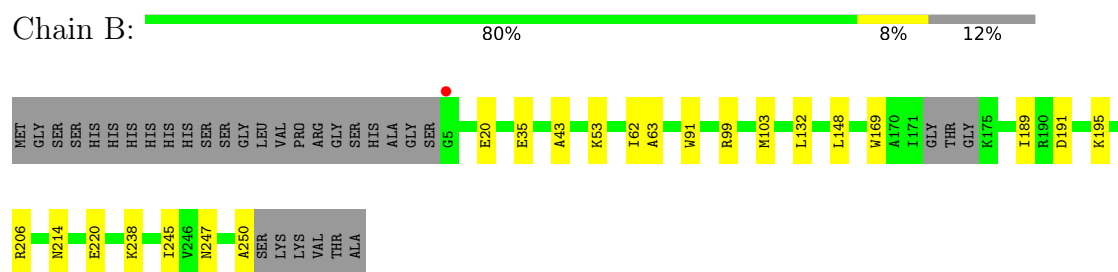
3 Residue-property plots

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.

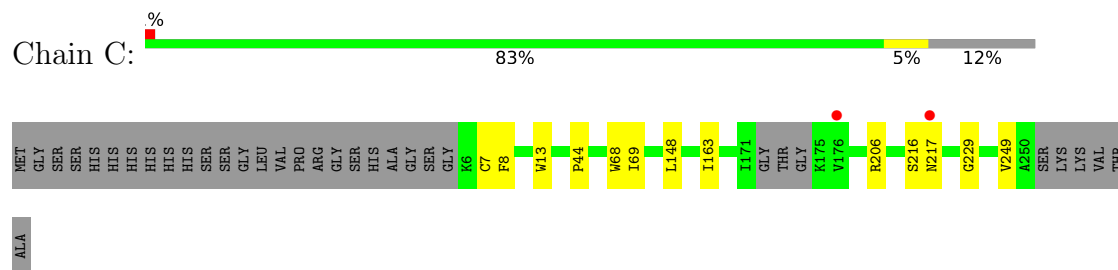
- Molecule 1: Triosephosphate isomerase



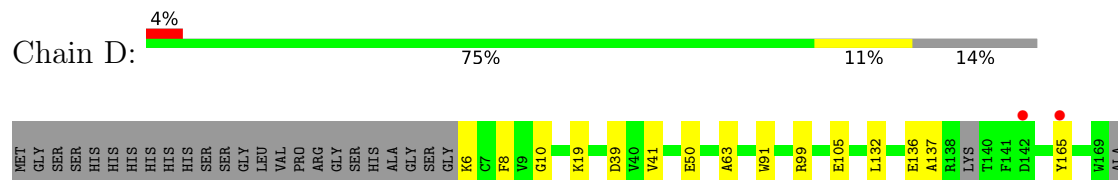
- Molecule 1: Triosephosphate isomerase

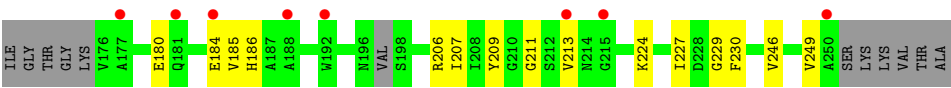


- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.95Å 82.12Å 154.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.97 – 1.90 44.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.97-1.90) 97.5 (44.97-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.185 , 0.235 0.185 , 0.234	Depositor DCC
R_{free} test set	2000 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7966	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 13.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.42	0/1857	0.57	1/2520 (0.0%)
1	B	0.42	0/1823	0.56	0/2474
1	C	0.38	0/1791	0.53	0/2437
1	D	0.37	0/1721	0.53	0/2337
All	All	0.40	0/7192	0.55	1/9768 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	GLU	CA-CB-CG	6.06	126.73	113.40

There are no chirality outliers.

There are no planarity outliers.

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	1823	0	1784	10	0
1	B	1790	0	1727	14	0
1	C	1758	0	1654	7	0
1	D	1692	0	1578	17	0
2	A	4	0	3	7	0
2	C	4	3	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	283	0	0	6	1
3	B	273	0	0	2	0
3	C	186	0	0	1	1
3	D	150	0	0	1	0
All	All	7963	3	6749	52	2

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 (52) 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:35:GLU:HG2	1:B:247:ASN:OD1	1.82	0.77
1:A:234:GLY:H	2:A:301:ACT:H3	1.50	0.75
1:A:234:GLY:H	2:A:301:ACT:CH3	2.00	0.75
1:A:216:SER:O	3:A:401:HOH:O	2.11	0.68
3:C:550:HOH:O	1:D:50:GLU:HG2	1.92	0.68
1:B:191:ASP:OD2	1:B:195:LYS:HE2	1.96	0.66
1:C:7:CYS:HB3	1:C:249:VAL:HG11	1.80	0.63
1:D:211:GLY:O	1:D:213:VAL:HG23	1.98	0.62
1:D:180:GLU:O	1:D:184:GLU:HG3	1.99	0.61
1:B:148:LEU:HD11	1:B:189:ILE:HG23	1.85	0.58
1:D:246:VAL:O	1:D:249:VAL:HG22	2.06	0.56
1:D:224:LYS:HB2	1:D:227:ILE:HD12	1.87	0.56
1:D:186:HIS:CD2	1:D:207:ILE:HG22	2.40	0.56
1:C:7:CYS:HB3	1:C:249:VAL:CG1	2.38	0.54
1:A:167:PRO:HD2	1:A:210:GLY:O	2.10	0.51
1:D:209:TYR:CZ	1:D:211:GLY:HA3	2.45	0.51
1:D:132:LEU:O	1:D:136:GLU:HG2	2.10	0.51
1:B:20:GLU:OE2	3:B:301:HOH:O	2.18	0.50
1:D:165:TYR:CE1	1:D:185:VAL:HG11	2.47	0.50
1:B:220:GLU:HB2	3:B:317:HOH:O	2.11	0.50
1:D:99:ARG:O	1:D:105:GLU:HG3	2.12	0.50
1:D:8:PHE:O	1:D:229:GLY:HA3	2.12	0.49
1:A:148:LEU:HD11	1:A:189:ILE:HG23	1.93	0.49
1:A:167:PRO:HG2	1:A:170:ALA:HB3	1.96	0.47
1:B:53:LYS:HA	1:B:62:ILE:HD11	1.97	0.47
1:A:53:LYS:HE2	3:A:624:HOH:O	2.14	0.47
1:D:6:LYS:O	1:D:206:ARG:HD3	2.15	0.47
1:C:148:LEU:HD21	1:C:163:ILE:HD13	1.97	0.47
1:C:216:SER:O	1:C:217:ASN:CB	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ALA:HB2	1:D:91:TRP:HB2	1.98	0.46
2:A:301:ACT:H2	3:A:442:HOH:O	2.15	0.46
2:A:301:ACT:H3	3:A:637:HOH:O	2.16	0.46
1:B:43:ALA:HA	1:B:63:ALA:O	2.17	0.45
1:C:68:TRP:CE2	1:C:69:ILE:HG12	2.52	0.45
1:B:214:ASN:HA	1:B:245:ILE:HD11	1.98	0.45
1:A:8:PHE:O	1:A:229:GLY:HA3	2.17	0.44
2:A:301:ACT:CH3	3:A:442:HOH:O	2.66	0.44
1:B:99:ARG:HA	1:B:103:MET:HB2	2.00	0.44
1:D:39:ASP:OD2	1:D:206:ARG:NH1	2.46	0.44
1:A:234:GLY:H	2:A:301:ACT:H2	1.82	0.43
1:D:19:LYS:HE3	3:D:416:HOH:O	2.16	0.43
1:B:35:GLU:HG3	1:B:250:ALA:CB	2.49	0.43
1:D:213:VAL:HG21	1:D:230:PHE:HD2	1.84	0.43
1:C:13:TRP:CZ3	1:C:44:PRO:HB3	2.55	0.42
1:A:178:THR:OG1	1:A:181:GLN:HG3	2.20	0.41
2:A:301:ACT:CH3	3:A:637:HOH:O	2.69	0.41
1:C:8:PHE:O	1:C:229:GLY:HA3	2.20	0.41
1:B:238:LYS:HE3	1:B:238:LYS:HB2	1.66	0.41
1:D:10:GLY:HA2	1:D:41:VAL:O	2.20	0.41
1:B:132:LEU:HA	1:B:169:TRP:CB	2.50	0.41
1:B:35:GLU:HG3	1:B:250:ALA:HB3	2.03	0.40
1:B:63:ALA:HB2	1:B:91:TRP:HB2	2.04	0.40

All (2) 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)
3:C:439:HOH:O	3:C:524:HOH:O[3_645]	2.08	0.12
3:A:414:HOH:O	3:A:486:HOH:O[4_455]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	244/275 (89%)	237 (97%)	6 (2%)	1 (0%)	34	24
1	B	239/275 (87%)	234 (98%)	5 (2%)	0	100	100
1	C	238/275 (86%)	231 (97%)	7 (3%)	0	100	100
1	D	229/275 (83%)	223 (97%)	5 (2%)	1 (0%)	34	24
All	All	950/1100 (86%)	925 (97%)	23 (2%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	137	ALA
1	A	249	VAL

5.3.2 Protein sidechains ⓘ

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	187/221 (85%)	186 (100%)	1 (0%)	88	89
1	B	181/221 (82%)	180 (99%)	1 (1%)	86	87
1	C	173/221 (78%)	172 (99%)	1 (1%)	86	87
1	D	163/221 (74%)	163 (100%)	0	100	100
All	All	704/884 (80%)	701 (100%)	3 (0%)	91	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ARG
1	B	206	ARG
1	C	206	ARG

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

Mol	Chain	Res	Type
1	A	146	GLN
1	B	146	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	ACT	A	301	-	3,3,3	1.25	0	3,3,3	1.35	0
2	ACT	C	301	-	3,3,3	1.08	0	3,3,3	1.79	1 (33%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	301	ACT	O-C-CH3	-2.35	113.17	122.33

There are no chirality outliers.

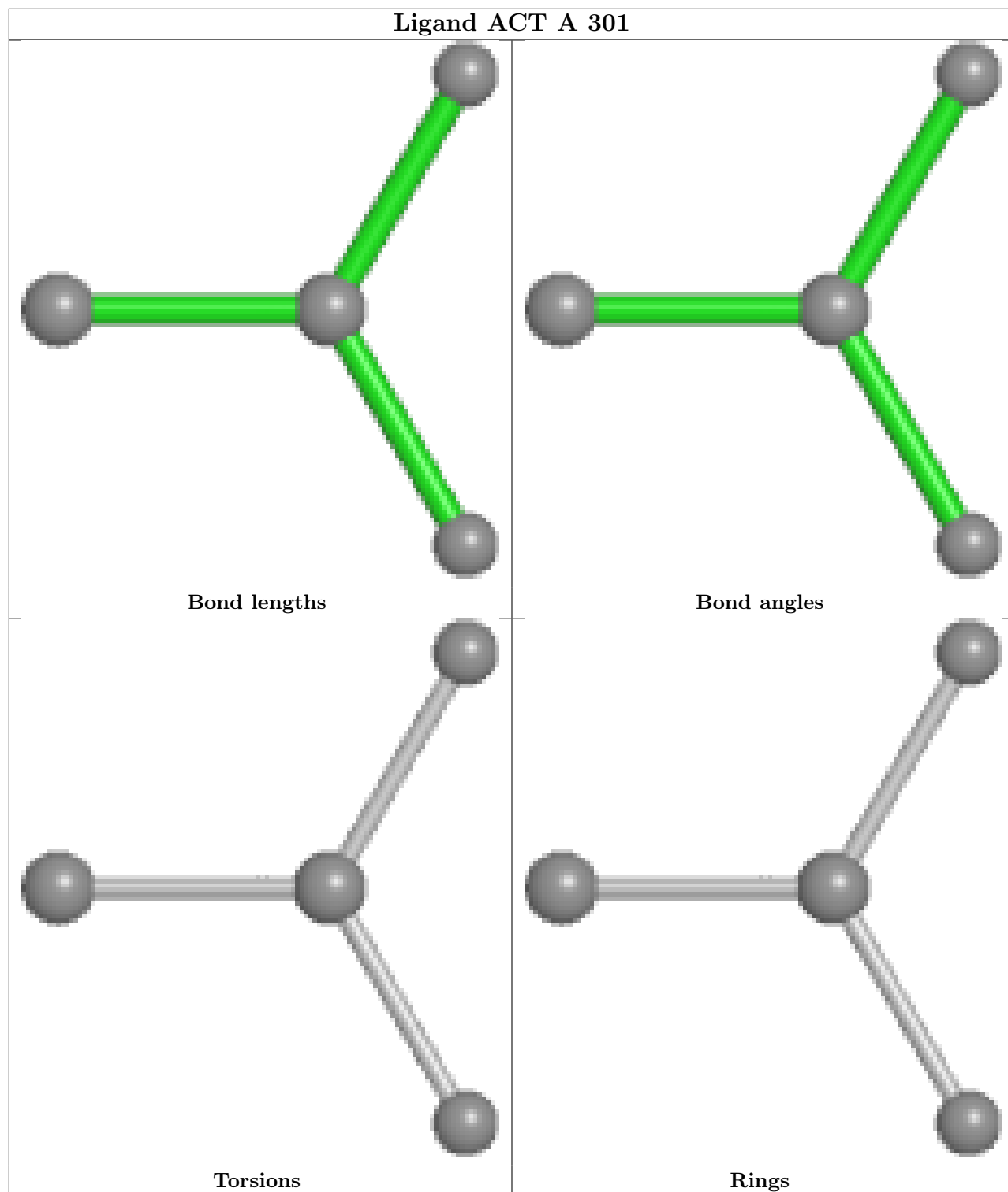
There are no torsion outliers.

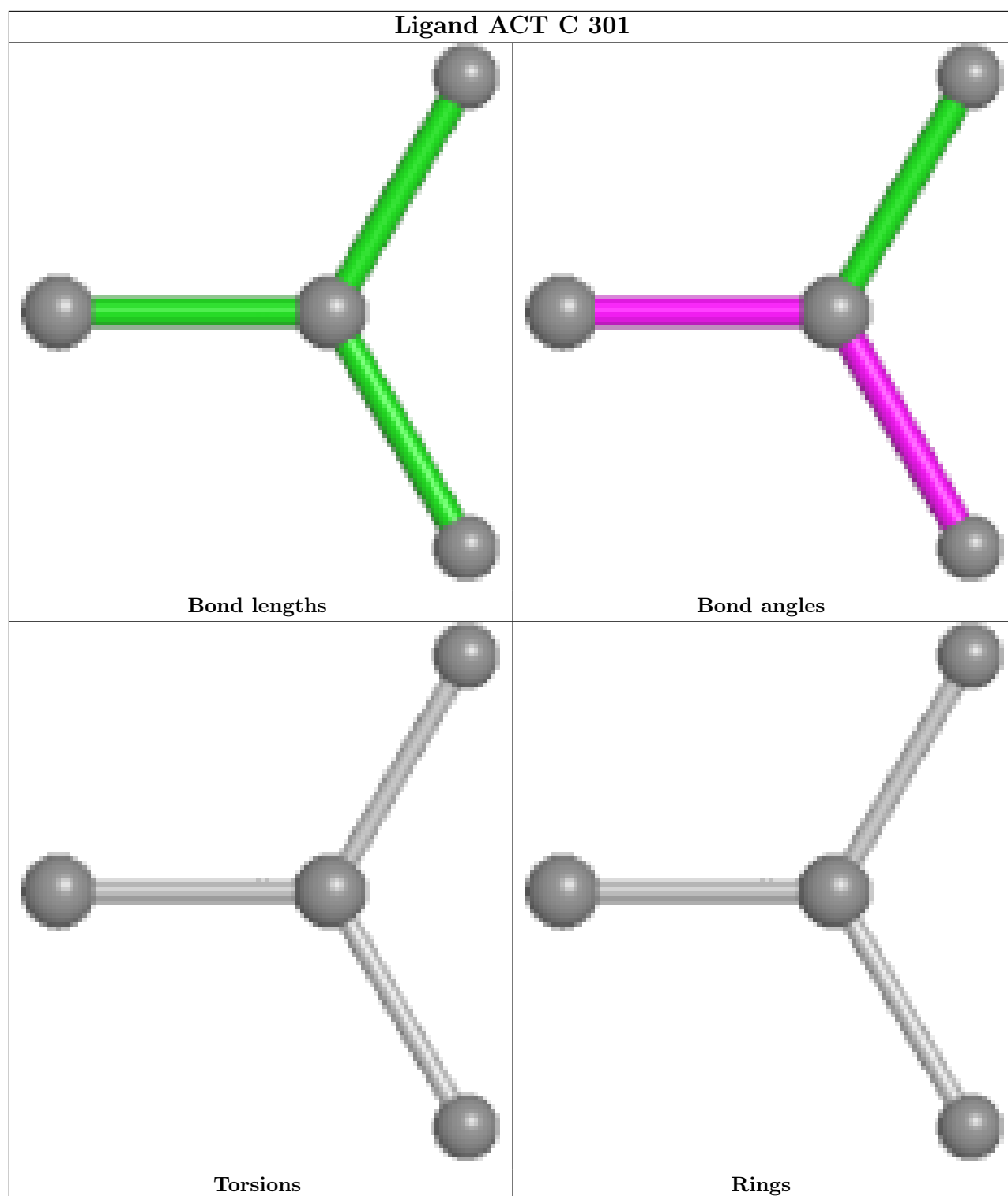
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ACT	7	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 than 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.





5.7 Other polymers [i](#)

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, 95th 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	246/275 (89%)	-0.12	7 (2%) 53 56	12, 21, 36, 46	0
1	B	243/275 (88%)	-0.27	1 (0%) 92 93	13, 22, 37, 55	0
1	C	242/275 (88%)	-0.02	2 (0%) 86 87	16, 27, 42, 50	0
1	D	237/275 (86%)	0.29	10 (4%) 36 39	17, 31, 51, 61	0
All	All	968/1100 (88%)	-0.03	20 (2%) 63 66	12, 25, 46, 61	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	ALA	4.9
1	A	171	ILE	4.9
1	A	177	ALA	4.7
1	A	176	VAL	4.4
1	D	215	GLY	3.8
1	A	5	GLY	3.0
1	D	165	TYR	3.0
1	B	5	GLY	2.8
1	D	142	ASP	2.8
1	D	181	GLN	2.6
1	D	177	ALA	2.6
1	D	213	VAL	2.6
1	D	184	GLU	2.5
1	C	217	ASN	2.4
1	A	174	GLY	2.4
1	D	188	ALA	2.4
1	D	192	TRP	2.3
1	A	173	THR	2.3
1	C	176	VAL	2.2
1	D	250	ALA	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](#)

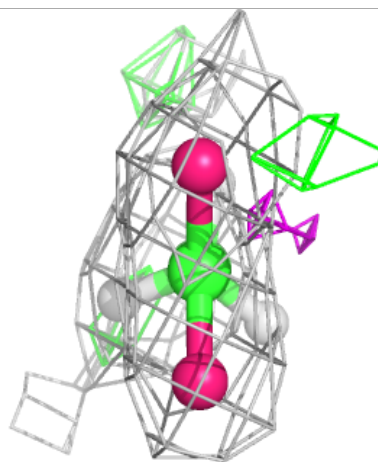
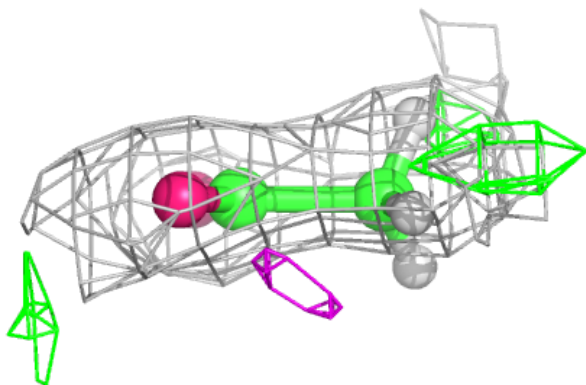
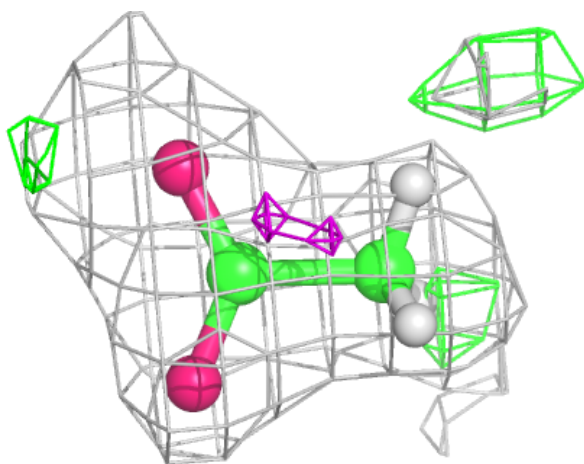
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ACT	C	301	4/4	0.72	0.34	39,44,47,47	0
2	ACT	A	301	4/4	0.91	0.15	20,22,33,33	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.

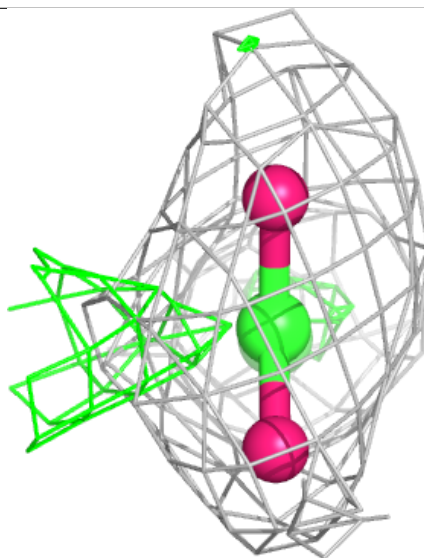
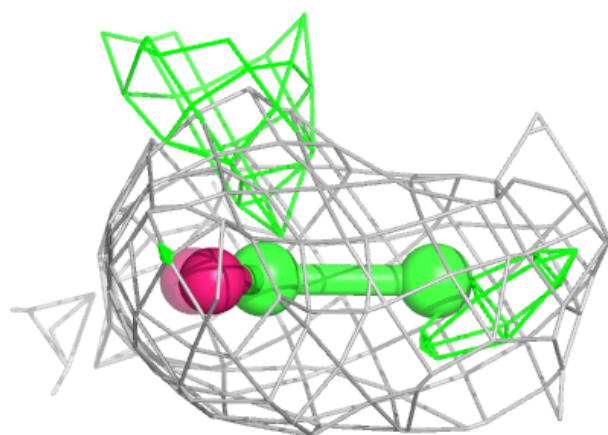
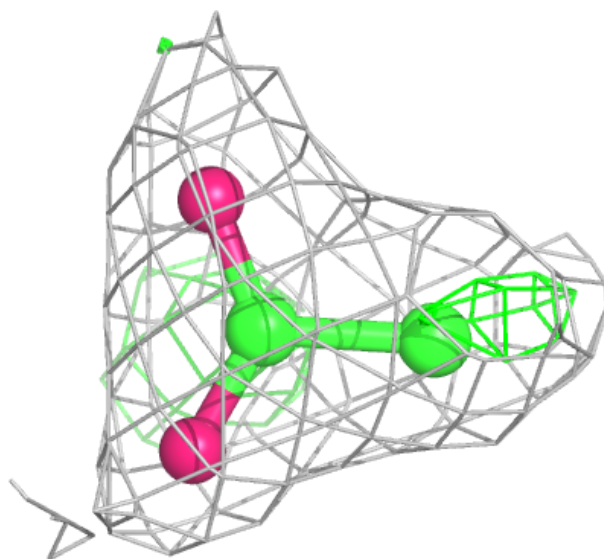
Electron density around ACT C 301:

$2mF_o-DF_c$ (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.