



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 11:31 AM EDT

PDB ID : 6SU1  
Title : Trypanosoma congolense pyruvate kinase in complex with citrate and glycerol  
Authors : Sterckx, Y.G.-J.; Pinto Torres, J.E.  
Deposited on : 2019-09-12  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

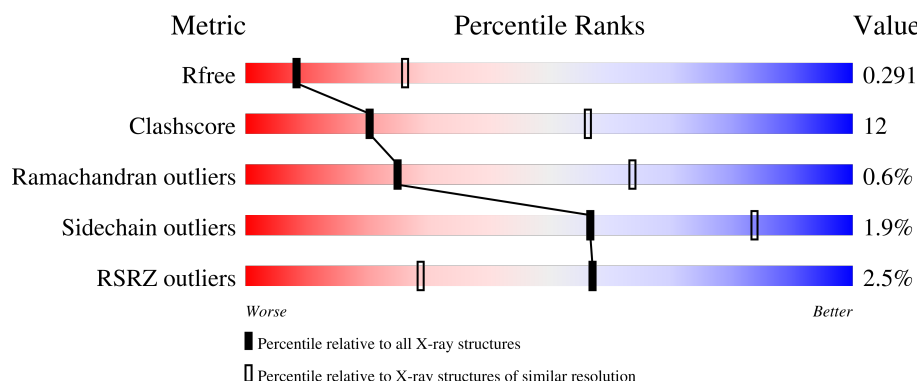
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	514	<div> <div>3%</div> <div>69%</div> <div>16%</div> <div>15%</div> </div>
1	B	514	<div> <div>5%</div> <div>74%</div> <div>18%</div> <div>7%</div> </div>
1	C	514	<div> <div>77%</div> <div>19%</div> <div>• •</div> </div>
1	D	514	<div> <div>3%</div> <div>74%</div> <div>22%</div> <div>• •</div> </div>
1	E	514	<div> <div>%</div> <div>74%</div> <div>22%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	514	
1	G	514	
1	H	514	

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
3	CIT	H	601	-	X	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 28228 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3226	2010	567	625	24			
1	B	476	Total	C	N	O	S	0	0	0
			3481	2164	623	667	27			
1	C	499	Total	C	N	O	S	0	1	0
			3726	2320	659	721	26			
1	D	498	Total	C	N	O	S	0	1	0
			3709	2306	660	717	26			
1	E	495	Total	C	N	O	S	0	0	0
			3710	2311	655	718	26			
1	F	498	Total	C	N	O	S	0	1	0
			3716	2316	658	716	26			
1	G	411	Total	C	N	O	S	0	1	0
			3054	1894	548	588	24			
1	H	449	Total	C	N	O	S	0	0	0
			3273	2029	586	635	23			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	GLU	-	expression tag	UNP G0UYF4
A	501	ASN	-	expression tag	UNP G0UYF4
A	502	LEU	-	expression tag	UNP G0UYF4
A	503	TYR	-	expression tag	UNP G0UYF4
A	504	PHE	-	expression tag	UNP G0UYF4
A	505	GLN	-	expression tag	UNP G0UYF4
A	506	SER	-	expression tag	UNP G0UYF4
A	507	GLY	-	expression tag	UNP G0UYF4
A	508	GLY	-	expression tag	UNP G0UYF4
A	509	HIS	-	expression tag	UNP G0UYF4
A	510	HIS	-	expression tag	UNP G0UYF4
A	511	HIS	-	expression tag	UNP G0UYF4
A	512	HIS	-	expression tag	UNP G0UYF4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	513	HIS	-	expression tag	UNP G0UYF4
A	514	HIS	-	expression tag	UNP G0UYF4
B	500	GLU	-	expression tag	UNP G0UYF4
B	501	ASN	-	expression tag	UNP G0UYF4
B	502	LEU	-	expression tag	UNP G0UYF4
B	503	TYR	-	expression tag	UNP G0UYF4
B	504	PHE	-	expression tag	UNP G0UYF4
B	505	GLN	-	expression tag	UNP G0UYF4
B	506	SER	-	expression tag	UNP G0UYF4
B	507	GLY	-	expression tag	UNP G0UYF4
B	508	GLY	-	expression tag	UNP G0UYF4
B	509	HIS	-	expression tag	UNP G0UYF4
B	510	HIS	-	expression tag	UNP G0UYF4
B	511	HIS	-	expression tag	UNP G0UYF4
B	512	HIS	-	expression tag	UNP G0UYF4
B	513	HIS	-	expression tag	UNP G0UYF4
B	514	HIS	-	expression tag	UNP G0UYF4
C	500	GLU	-	expression tag	UNP G0UYF4
C	501	ASN	-	expression tag	UNP G0UYF4
C	502	LEU	-	expression tag	UNP G0UYF4
C	503	TYR	-	expression tag	UNP G0UYF4
C	504	PHE	-	expression tag	UNP G0UYF4
C	505	GLN	-	expression tag	UNP G0UYF4
C	506	SER	-	expression tag	UNP G0UYF4
C	507	GLY	-	expression tag	UNP G0UYF4
C	508	GLY	-	expression tag	UNP G0UYF4
C	509	HIS	-	expression tag	UNP G0UYF4
C	510	HIS	-	expression tag	UNP G0UYF4
C	511	HIS	-	expression tag	UNP G0UYF4
C	512	HIS	-	expression tag	UNP G0UYF4
C	513	HIS	-	expression tag	UNP G0UYF4
C	514	HIS	-	expression tag	UNP G0UYF4
D	500	GLU	-	expression tag	UNP G0UYF4
D	501	ASN	-	expression tag	UNP G0UYF4
D	502	LEU	-	expression tag	UNP G0UYF4
D	503	TYR	-	expression tag	UNP G0UYF4
D	504	PHE	-	expression tag	UNP G0UYF4
D	505	GLN	-	expression tag	UNP G0UYF4
D	506	SER	-	expression tag	UNP G0UYF4
D	507	GLY	-	expression tag	UNP G0UYF4
D	508	GLY	-	expression tag	UNP G0UYF4
D	509	HIS	-	expression tag	UNP G0UYF4

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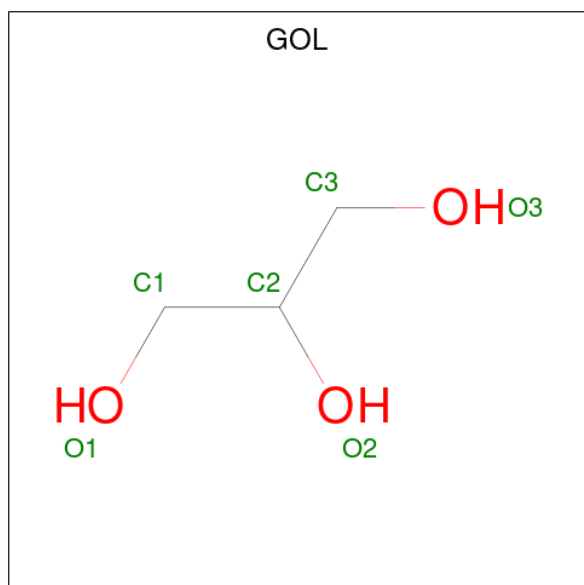
Chain	Residue	Modelled	Actual	Comment	Reference
D	510	HIS	-	expression tag	UNP G0UYF4
D	511	HIS	-	expression tag	UNP G0UYF4
D	512	HIS	-	expression tag	UNP G0UYF4
D	513	HIS	-	expression tag	UNP G0UYF4
D	514	HIS	-	expression tag	UNP G0UYF4
E	500	GLU	-	expression tag	UNP G0UYF4
E	501	ASN	-	expression tag	UNP G0UYF4
E	502	LEU	-	expression tag	UNP G0UYF4
E	503	TYR	-	expression tag	UNP G0UYF4
E	504	PHE	-	expression tag	UNP G0UYF4
E	505	GLN	-	expression tag	UNP G0UYF4
E	506	SER	-	expression tag	UNP G0UYF4
E	507	GLY	-	expression tag	UNP G0UYF4
E	508	GLY	-	expression tag	UNP G0UYF4
E	509	HIS	-	expression tag	UNP G0UYF4
E	510	HIS	-	expression tag	UNP G0UYF4
E	511	HIS	-	expression tag	UNP G0UYF4
E	512	HIS	-	expression tag	UNP G0UYF4
E	513	HIS	-	expression tag	UNP G0UYF4
E	514	HIS	-	expression tag	UNP G0UYF4
F	500	GLU	-	expression tag	UNP G0UYF4
F	501	ASN	-	expression tag	UNP G0UYF4
F	502	LEU	-	expression tag	UNP G0UYF4
F	503	TYR	-	expression tag	UNP G0UYF4
F	504	PHE	-	expression tag	UNP G0UYF4
F	505	GLN	-	expression tag	UNP G0UYF4
F	506	SER	-	expression tag	UNP G0UYF4
F	507	GLY	-	expression tag	UNP G0UYF4
F	508	GLY	-	expression tag	UNP G0UYF4
F	509	HIS	-	expression tag	UNP G0UYF4
F	510	HIS	-	expression tag	UNP G0UYF4
F	511	HIS	-	expression tag	UNP G0UYF4
F	512	HIS	-	expression tag	UNP G0UYF4
F	513	HIS	-	expression tag	UNP G0UYF4
F	514	HIS	-	expression tag	UNP G0UYF4
G	500	GLU	-	expression tag	UNP G0UYF4
G	501	ASN	-	expression tag	UNP G0UYF4
G	502	LEU	-	expression tag	UNP G0UYF4
G	503	TYR	-	expression tag	UNP G0UYF4
G	504	PHE	-	expression tag	UNP G0UYF4
G	505	GLN	-	expression tag	UNP G0UYF4
G	506	SER	-	expression tag	UNP G0UYF4

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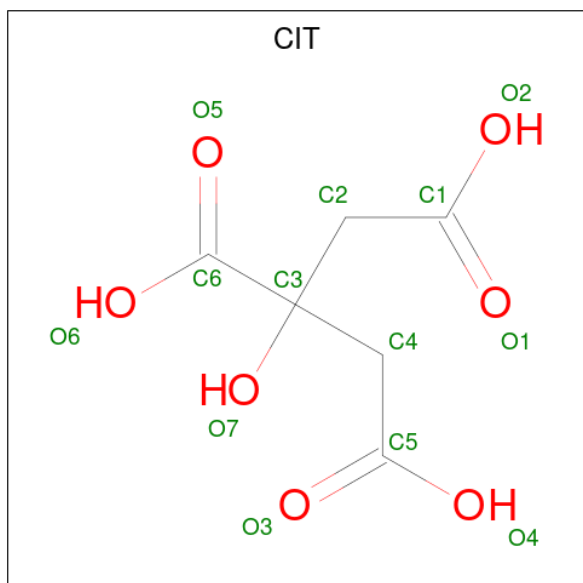
Chain	Residue	Modelled	Actual	Comment	Reference
G	507	GLY	-	expression tag	UNP G0UYF4
G	508	GLY	-	expression tag	UNP G0UYF4
G	509	HIS	-	expression tag	UNP G0UYF4
G	510	HIS	-	expression tag	UNP G0UYF4
G	511	HIS	-	expression tag	UNP G0UYF4
G	512	HIS	-	expression tag	UNP G0UYF4
G	513	HIS	-	expression tag	UNP G0UYF4
G	514	HIS	-	expression tag	UNP G0UYF4
H	500	GLU	-	expression tag	UNP G0UYF4
H	501	ASN	-	expression tag	UNP G0UYF4
H	502	LEU	-	expression tag	UNP G0UYF4
H	503	TYR	-	expression tag	UNP G0UYF4
H	504	PHE	-	expression tag	UNP G0UYF4
H	505	GLN	-	expression tag	UNP G0UYF4
H	506	SER	-	expression tag	UNP G0UYF4
H	507	GLY	-	expression tag	UNP G0UYF4
H	508	GLY	-	expression tag	UNP G0UYF4
H	509	HIS	-	expression tag	UNP G0UYF4
H	510	HIS	-	expression tag	UNP G0UYF4
H	511	HIS	-	expression tag	UNP G0UYF4
H	512	HIS	-	expression tag	UNP G0UYF4
H	513	HIS	-	expression tag	UNP G0UYF4
H	514	HIS	-	expression tag	UNP G0UYF4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	6	7		

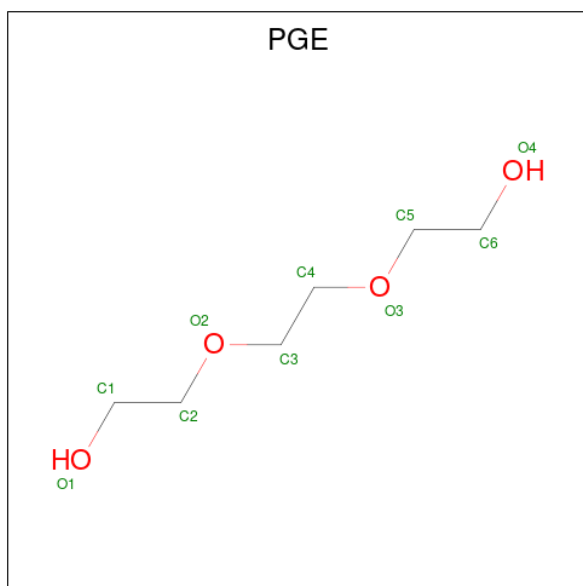
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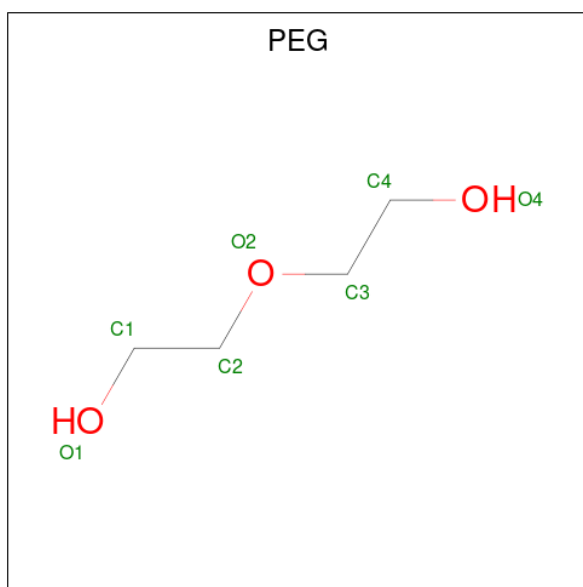
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		
3	H	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).




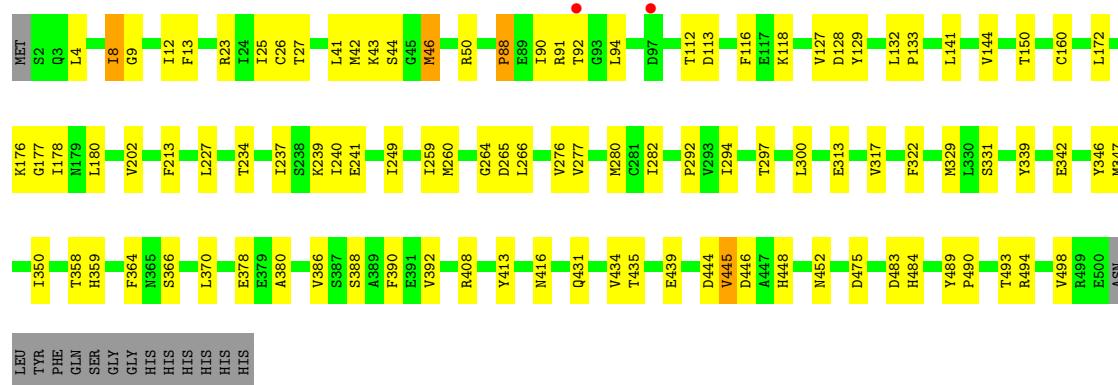
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	23	Total	O	0	0
			23	23		
6	C	32	Total	O	0	0
			32	32		
6	D	15	Total	O	0	0
			15	15		
6	E	22	Total	O	0	0
			22	22		
6	F	31	Total	O	0	0
			31	31		
6	G	20	Total	O	0	0
			20	20		
6	H	16	Total	O	0	0
			16	16		

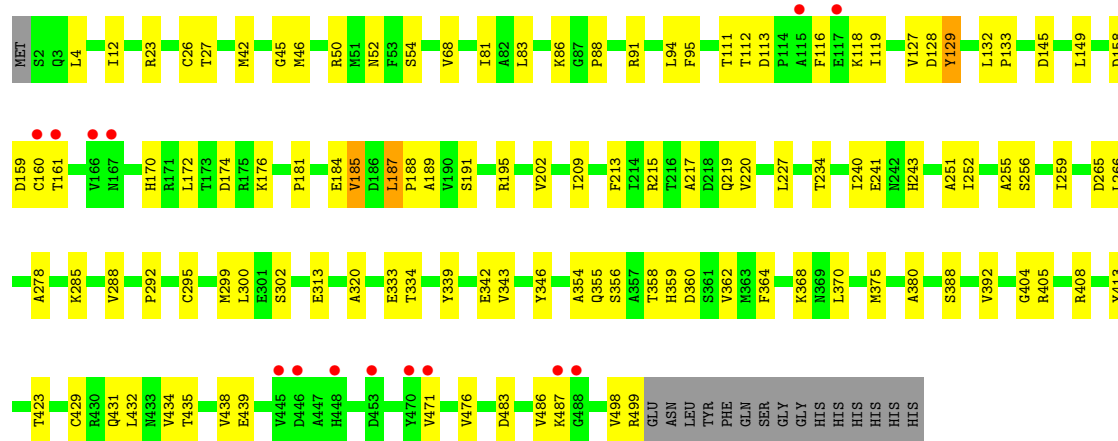


Chain C:  77% 19% ..




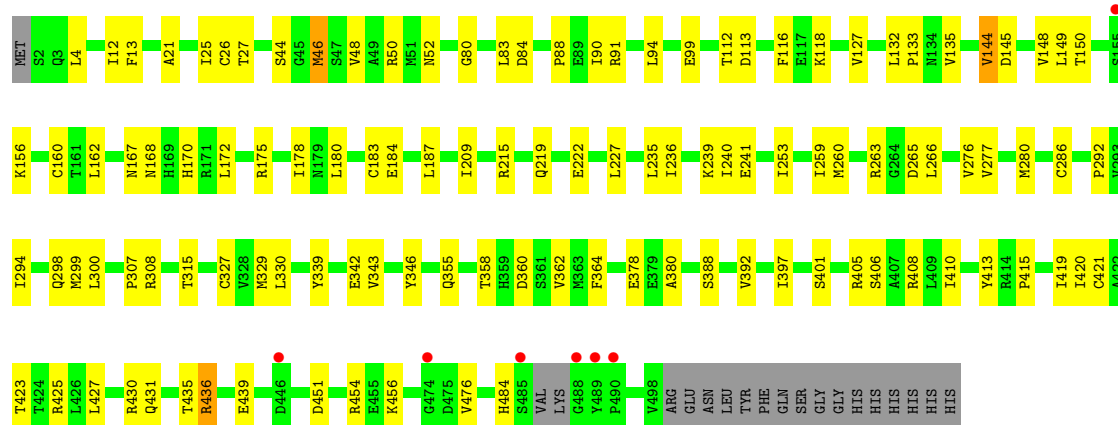
• Molecule 1: Pyruvate kinase

Chain D:  74% 22% ..



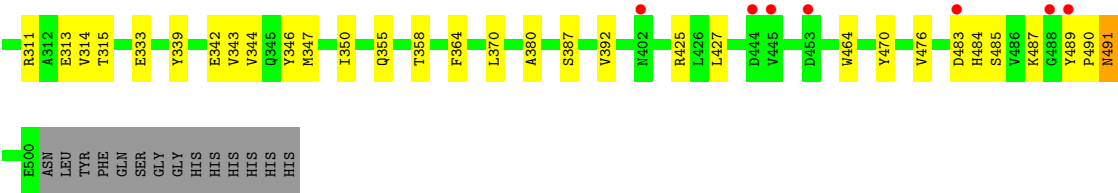
• Molecule 1: Pyruvate kinase

Chain E:  74% 22% ..



• Molecule 1: Pyruvate kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.45Å 107.15Å 148.00Å 109.74° 90.51° 106.78°	Depositor
Resolution (Å)	49.33 – 3.00 49.33 – 2.79	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.33-3.00) 92.8 (49.33-2.79)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.208 , 0.257 0.243 , 0.291	Depositor DCC
$R_{free}$ test set	5317 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.8	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 80.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	28228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PGE, PEG, CIT, GOL

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	0.51	0/3268	0.75	0/4440
1	B	0.55	0/3529	0.77	0/4792
1	C	0.53	0/3787	0.76	0/5150
1	D	0.48	0/3770	0.74	0/5130
1	E	0.50	0/3767	0.74	0/5117
1	F	0.51	0/3776	0.75	0/5133
1	G	0.53	0/3098	0.75	0/4201
1	H	0.48	0/3317	0.73	0/4515
All	All	0.51	0/28312	0.75	0/38478

There are no bond length outliers.

There are no bond angle outliers.

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	3226	0	3135	84	0
1	B	3481	0	3400	94	0
1	C	3726	0	3664	102	0
1	D	3709	0	3630	113	0
1	E	3710	0	3667	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3716	0	3671	90	0
1	G	3054	0	3026	80	0
1	H	3273	0	3139	81	0
2	A	12	0	16	1	0
2	B	6	0	8	0	0
2	C	12	0	16	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	2	0
2	G	6	0	8	1	0
2	H	6	0	8	1	0
3	B	13	0	5	4	0
3	C	13	0	5	1	0
3	D	13	0	5	1	0
3	E	13	0	5	0	0
3	F	13	0	5	0	0
3	H	13	0	5	3	0
4	F	10	0	14	0	0
5	F	7	0	10	0	0
6	A	19	0	0	0	0
6	B	23	0	0	0	0
6	C	32	0	0	2	0
6	D	15	0	0	0	0
6	E	22	0	0	0	0
6	F	31	0	0	0	0
6	G	20	0	0	0	0
6	H	16	0	0	0	0
All	All	28228	0	27466	689	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 12.

The worst 5 of 689 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:LEU:CD2	1:D:188:PRO:HD2	1.45	1.45
1:G:299:MET:CE	1:G:328:VAL:HG22	1.46	1.43
1:C:202:VAL:CG2	1:C:227:LEU:HD22	1.56	1.35
1:G:202:VAL:CG2	1:G:227:LEU:HD22	1.56	1.34
1:D:202:VAL:CG2	1:D:227:LEU:HD22	1.57	1.32

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	427/514 (83%)	387 (91%)	33 (8%)	7 (2%)	9	40
1	B	468/514 (91%)	429 (92%)	38 (8%)	1 (0%)	47	82
1	C	498/514 (97%)	454 (91%)	41 (8%)	3 (1%)	25	64
1	D	497/514 (97%)	457 (92%)	38 (8%)	2 (0%)	34	72
1	E	491/514 (96%)	466 (95%)	25 (5%)	0	100	100
1	F	497/514 (97%)	460 (93%)	36 (7%)	1 (0%)	47	82
1	G	408/514 (79%)	382 (94%)	24 (6%)	2 (0%)	29	68
1	H	437/514 (85%)	399 (91%)	33 (8%)	5 (1%)	14	50
All	All	3723/4112 (90%)	3434 (92%)	268 (7%)	21 (1%)	25	64

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	LYS
1	A	110	VAL
1	A	184	GLU
1	C	445	VAL
1	C	484	HIS

### 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	338/435 (78%)	335 (99%)	3 (1%)	78	92
1	B	364/435 (84%)	358 (98%)	6 (2%)	62	86
1	C	401/435 (92%)	394 (98%)	7 (2%)	60	85
1	D	397/435 (91%)	389 (98%)	8 (2%)	55	83
1	E	402/435 (92%)	394 (98%)	8 (2%)	55	83
1	F	400/435 (92%)	387 (97%)	13 (3%)	38	73
1	G	327/435 (75%)	324 (99%)	3 (1%)	78	92
1	H	340/435 (78%)	333 (98%)	7 (2%)	53	82
All	All	2969/3480 (85%)	2914 (98%)	55 (2%)	57	84

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	172	LEU
1	F	227	LEU
1	H	491	ASN
1	H	137	ARG
1	E	308	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	359	HIS
1	F	459	GLN
1	H	279	GLN
1	G	492	GLN
1	B	179	ASN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

18 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	GOL	H	602	-	5,5,5	0.06	0	5,5,5	0.35	0
3	CIT	H	601	-	12,12,12	1.95	6 (50%)	17,17,17	2.39	7 (41%)
2	GOL	D	602	-	5,5,5	0.12	0	5,5,5	0.29	0
4	PGE	F	603	-	9,9,9	0.16	0	8,8,8	0.12	0
2	GOL	F	602	-	5,5,5	0.09	0	5,5,5	0.70	0
2	GOL	A	601	-	5,5,5	0.14	0	5,5,5	0.46	0
2	GOL	A	602	-	5,5,5	0.15	0	5,5,5	0.30	0
2	GOL	C	602	-	5,5,5	0.11	0	5,5,5	0.31	0
2	GOL	B	602	-	5,5,5	0.11	0	5,5,5	0.23	0
2	GOL	G	601	-	5,5,5	0.08	0	5,5,5	0.28	0
3	CIT	E	601	-	12,12,12	1.85	6 (50%)	17,17,17	2.41	6 (35%)
3	CIT	F	601	-	12,12,12	0.30	0	17,17,17	0.89	1 (5%)
5	PEG	F	604	-	6,6,6	0.26	0	5,5,5	0.16	0
3	CIT	D	601	-	12,12,12	1.97	6 (50%)	17,17,17	2.39	8 (47%)
2	GOL	C	603	-	5,5,5	0.07	0	5,5,5	0.20	0
3	CIT	C	601	-	12,12,12	1.63	4 (33%)	17,17,17	1.53	4 (23%)
3	CIT	B	601	-	12,12,12	0.31	0	17,17,17	0.68	1 (5%)
2	GOL	E	602	-	5,5,5	0.10	0	5,5,5	0.18	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
2	GOL	H	602	-	-	1/4/4/4	-
3	CIT	H	601	-	-	5/16/16/16	-
2	GOL	D	602	-	-	0/4/4/4	-
4	PGE	F	603	-	-	3/7/7/7	-
2	GOL	F	602	-	-	1/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	C	602	-	-	0/4/4/4	-
2	GOL	B	602	-	-	0/4/4/4	-
2	GOL	G	601	-	-	3/4/4/4	-
3	CIT	E	601	-	-	0/16/16/16	-
3	CIT	F	601	-	-	5/16/16/16	-
5	PEG	F	604	-	-	1/4/4/4	-
3	CIT	D	601	-	-	0/16/16/16	-
2	GOL	C	603	-	-	0/4/4/4	-
3	CIT	C	601	-	-	0/16/16/16	-
3	CIT	B	601	-	-	3/16/16/16	-
2	GOL	E	602	-	-	0/4/4/4	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	CIT	O4-C5	-3.29	1.19	1.30
3	C	601	CIT	O1-C1	3.16	1.32	1.22
3	D	601	CIT	O5-C6	3.03	1.31	1.22
3	H	601	CIT	O5-C6	2.98	1.31	1.22
3	D	601	CIT	O1-C1	2.96	1.31	1.22

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	CIT	O6-C6-C3	5.34	123.39	113.14
3	H	601	CIT	O6-C6-C3	5.31	123.33	113.14
3	E	601	CIT	O6-C6-C3	5.09	122.91	113.14
3	E	601	CIT	O5-C6-C3	-4.69	113.00	122.09
3	D	601	CIT	O5-C6-C3	-4.59	113.19	122.09

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

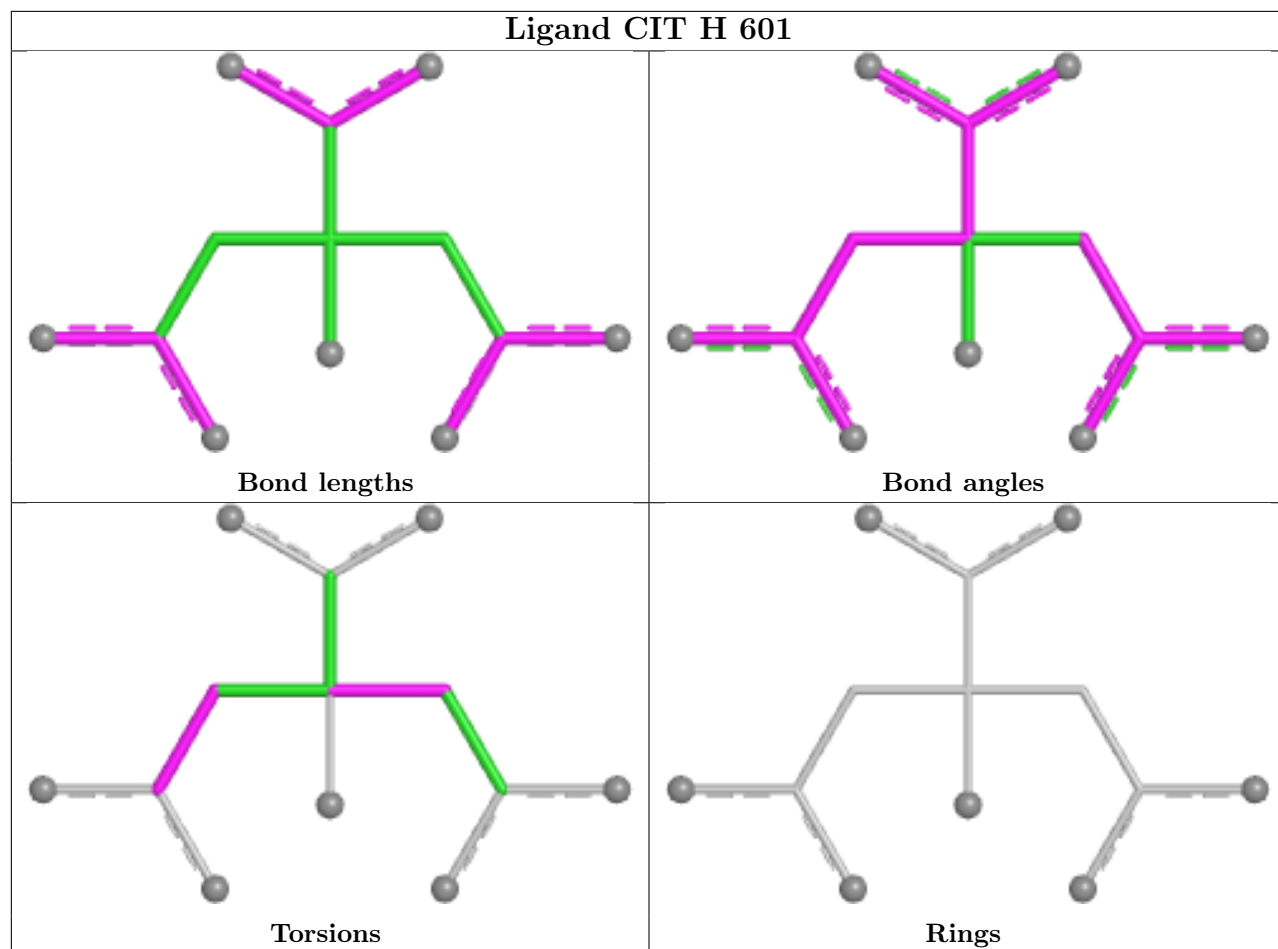
Mol	Chain	Res	Type	Atoms
2	A	602	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-C3
3	F	601	CIT	C1-C2-C3-O7
3	F	601	CIT	C1-C2-C3-C6
3	B	601	CIT	C1-C2-C3-O7

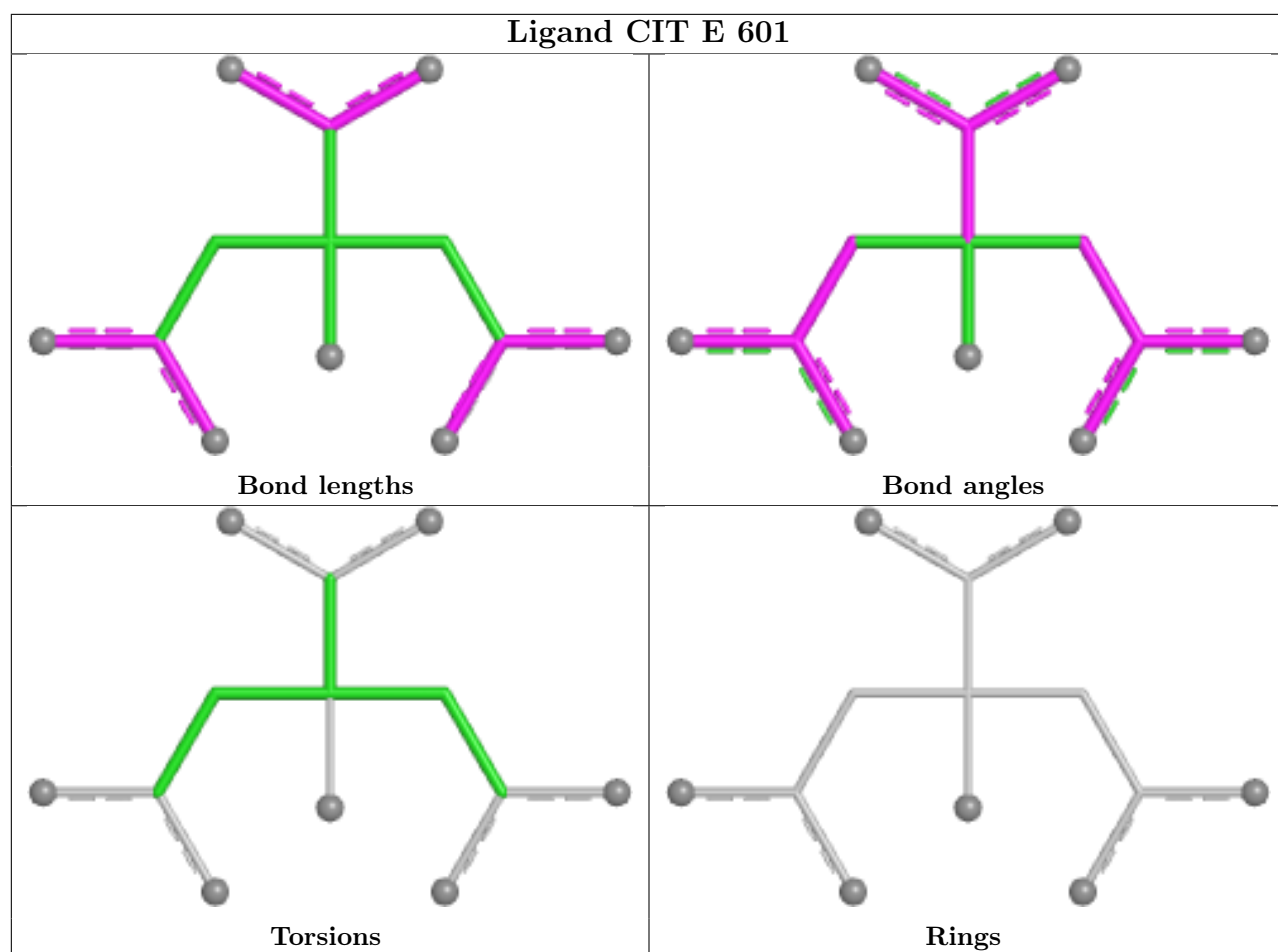
There are no ring outliers.

8 monomers are involved in 14 short contacts:

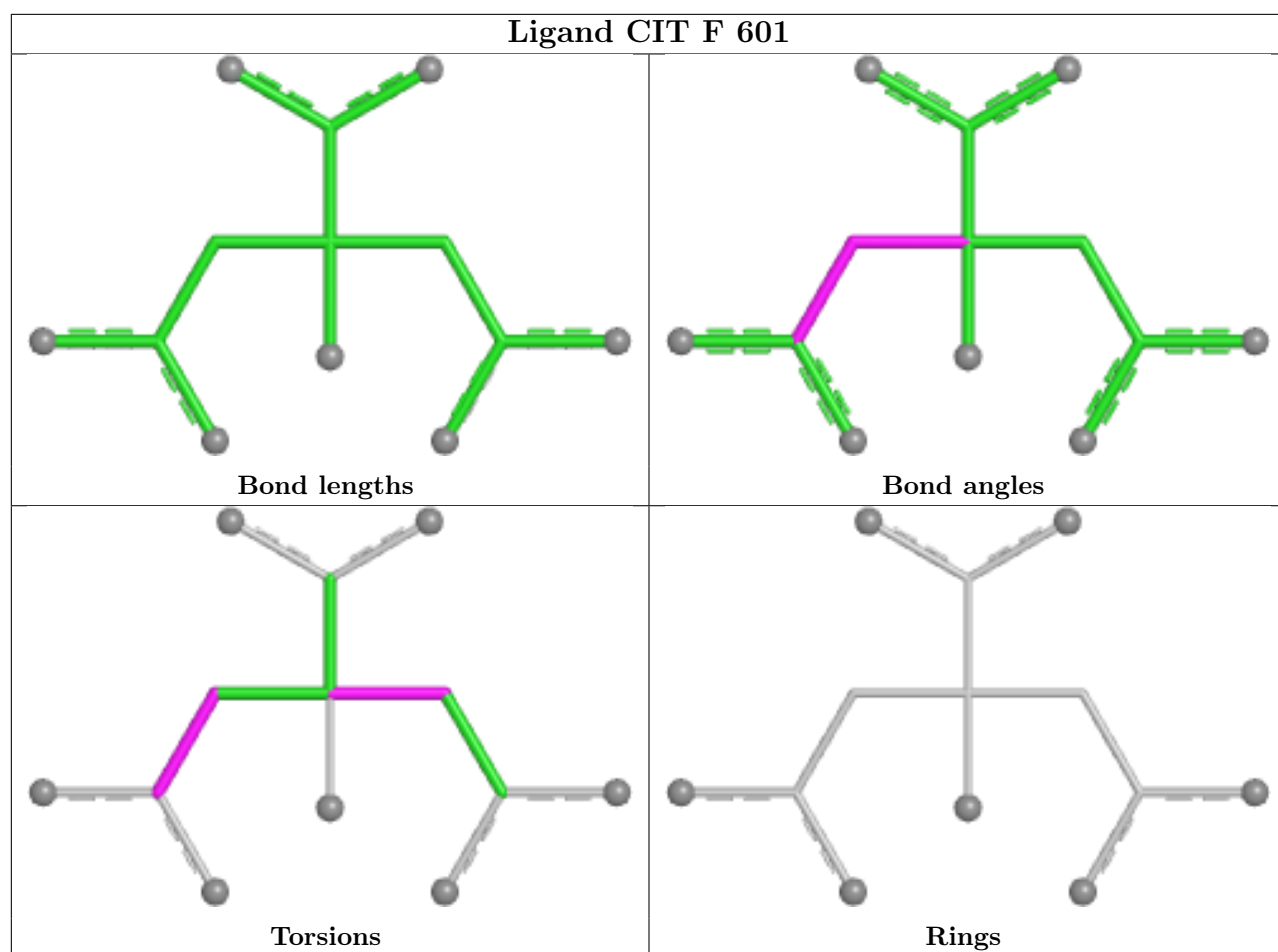
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	602	GOL	1	0
3	H	601	CIT	3	0
2	F	602	GOL	2	0
2	A	601	GOL	1	0
2	G	601	GOL	1	0
3	D	601	CIT	1	0
3	C	601	CIT	1	0
3	B	601	CIT	4	0

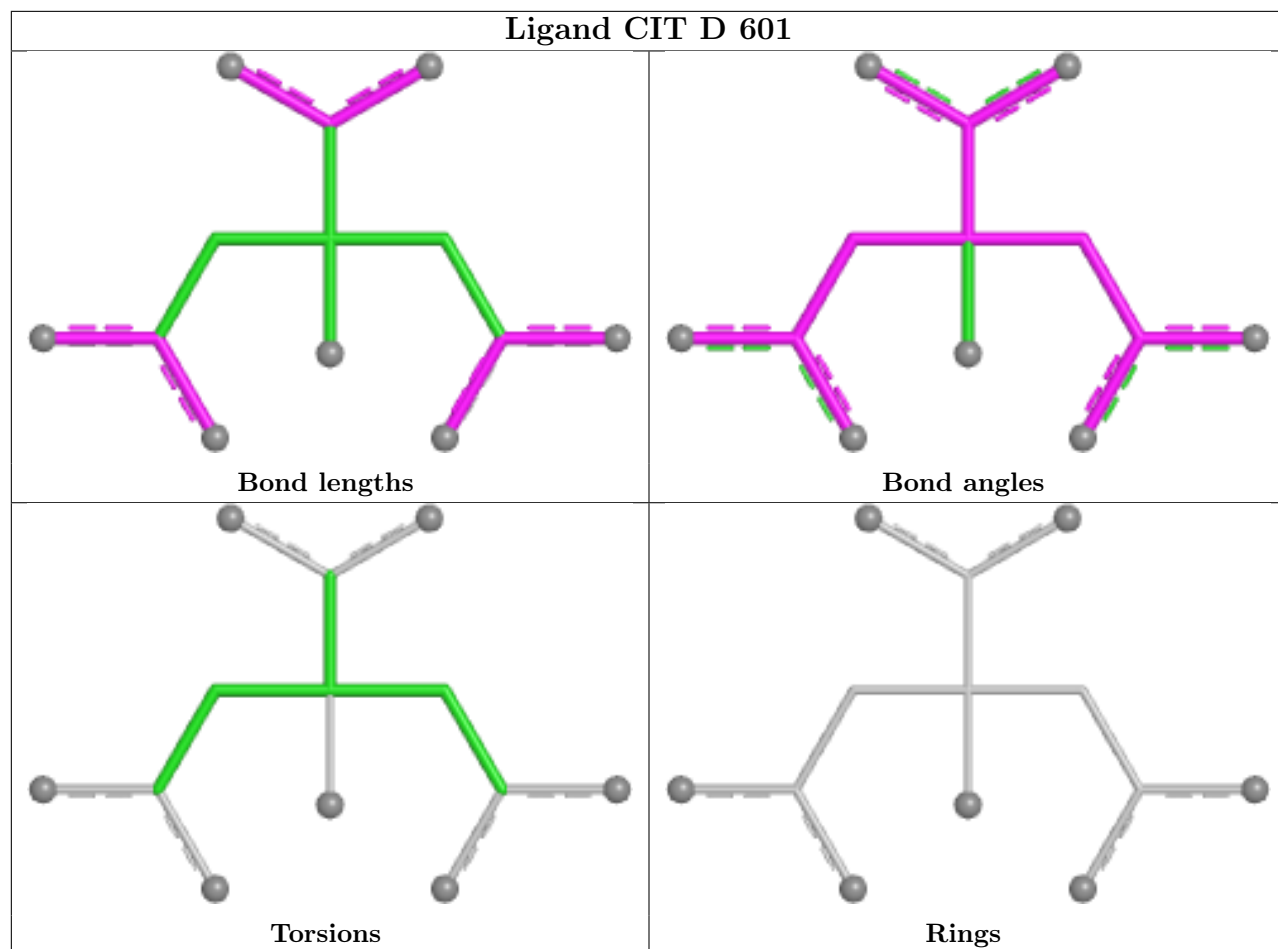
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

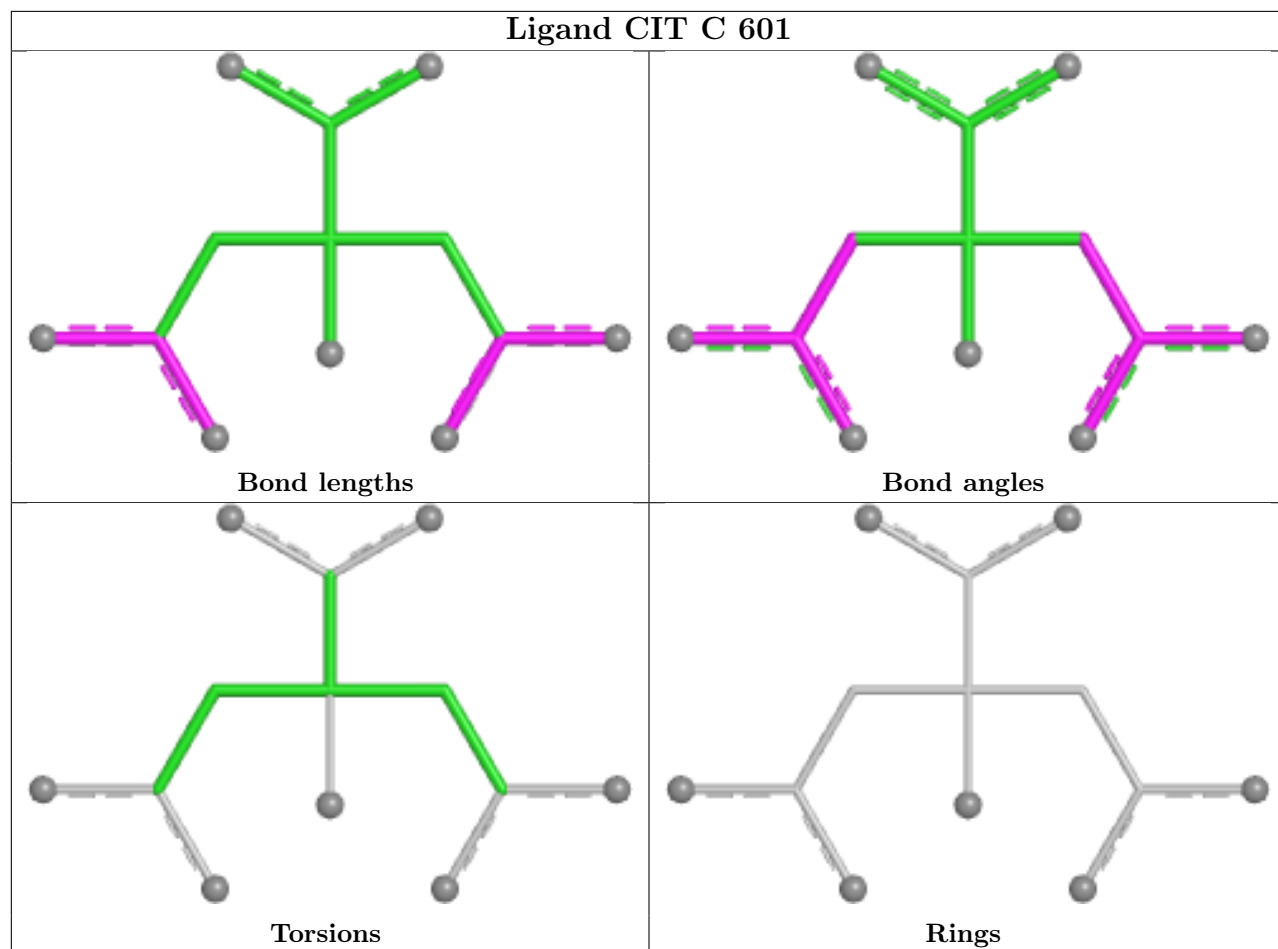


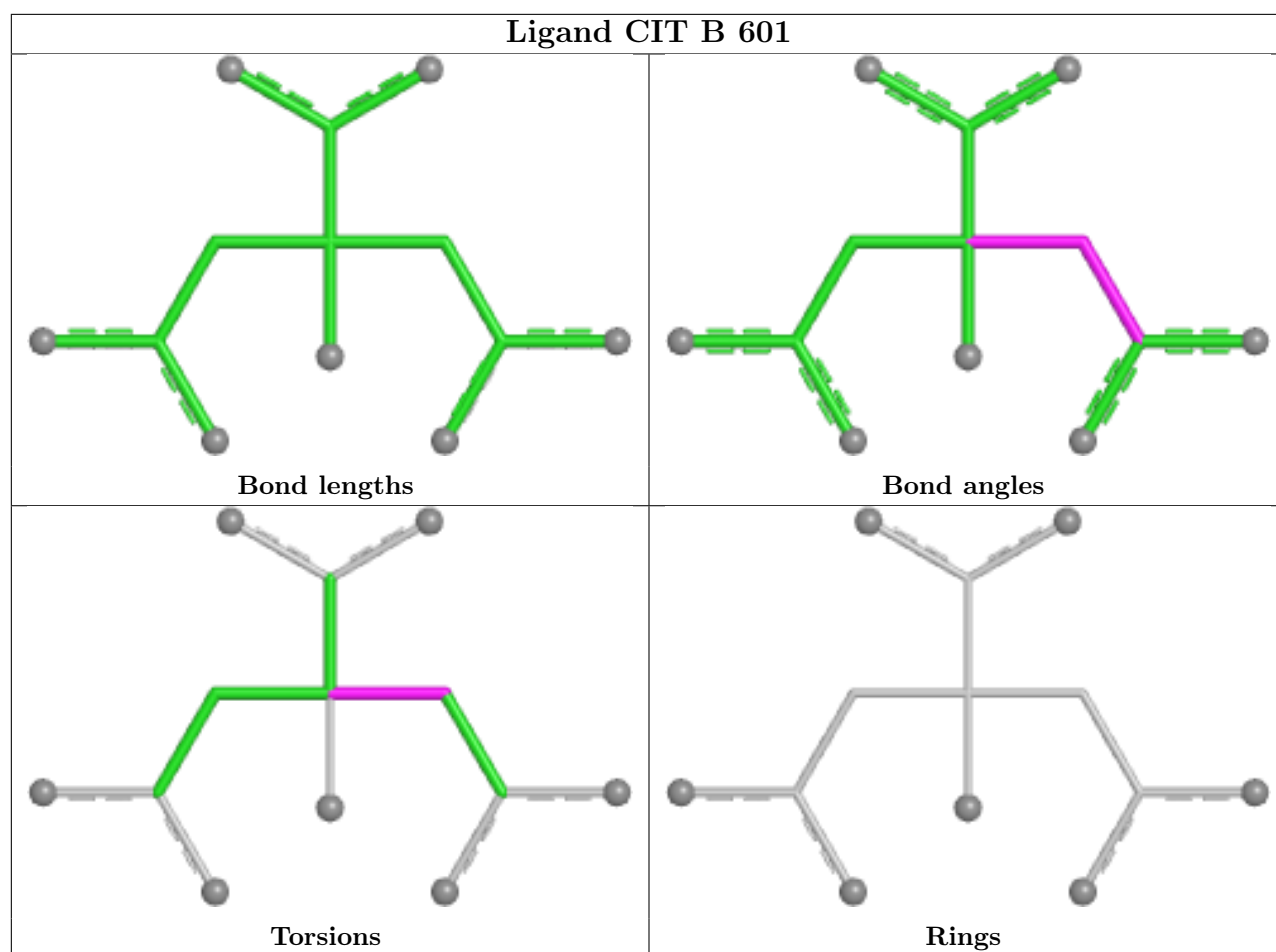












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	439/514 (85%)	-0.06	13 (2%)	50	22	51, 85, 134, 165	0
1	B	476/514 (92%)	-0.13	28 (5%)	22	7	41, 73, 174, 272	0
1	C	499/514 (97%)	-0.27	2 (0%)	92	79	48, 80, 110, 137	0
1	D	498/514 (96%)	-0.16	14 (2%)	53	25	56, 88, 133, 179	0
1	E	495/514 (96%)	-0.28	7 (1%)	75	49	56, 79, 112, 171	0
1	F	498/514 (96%)	-0.28	5 (1%)	82	59	47, 78, 107, 127	0
1	G	411/514 (79%)	-0.37	4 (0%)	82	59	49, 74, 115, 155	0
1	H	449/514 (87%)	0.10	20 (4%)	33	12	56, 103, 144, 175	0
All	All	3765/4112 (91%)	-0.18	93 (2%)	57	29	41, 82, 129, 272	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	488	GLY	8.8
1	H	402	ASN	6.5
1	B	164	CYS	6.4
1	A	144	VAL	6.1
1	A	151	LEU	4.9

### 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

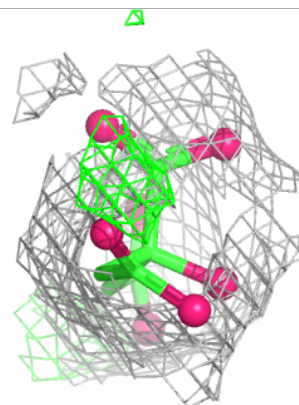
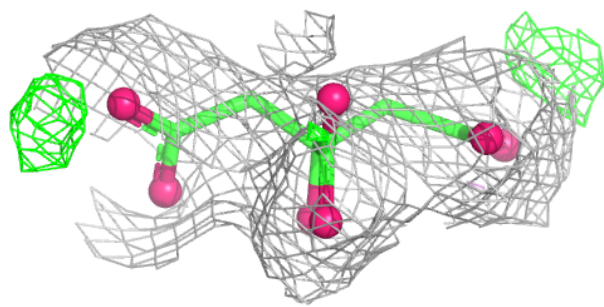
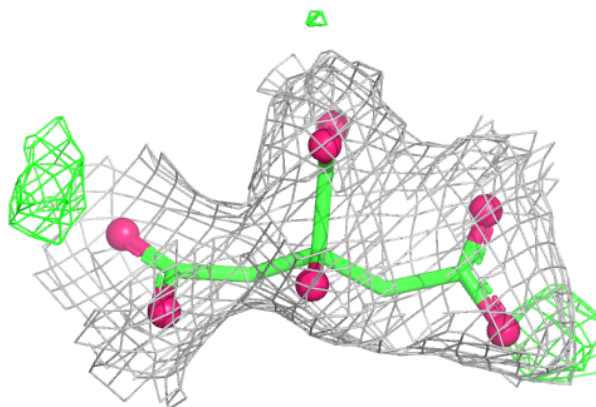
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CIT	D	601	13/13	0.58	0.33	112,123,127,128	0
2	GOL	F	602	6/6	0.75	0.18	85,88,89,91	0
4	PGE	F	603	10/10	0.78	0.21	90,98,101,101	0
3	CIT	H	601	13/13	0.80	0.29	141,145,149,150	0
3	CIT	F	601	13/13	0.81	0.20	101,109,117,117	0
2	GOL	A	602	6/6	0.83	0.16	76,80,81,81	0
3	CIT	C	601	13/13	0.83	0.35	96,105,108,110	0
2	GOL	G	601	6/6	0.85	0.14	88,89,89,90	0
5	PEG	F	604	7/7	0.85	0.16	83,84,87,87	0
2	GOL	B	602	6/6	0.86	0.20	80,82,84,85	0
3	CIT	B	601	13/13	0.88	0.16	107,121,124,127	0
2	GOL	C	602	6/6	0.89	0.14	91,93,93,94	0
2	GOL	C	603	6/6	0.90	0.19	85,89,89,89	0
2	GOL	A	601	6/6	0.90	0.15	59,67,68,69	0
2	GOL	E	602	6/6	0.91	0.13	71,79,82,82	0
2	GOL	D	602	6/6	0.92	0.25	76,80,83,84	0
3	CIT	E	601	13/13	0.92	0.18	103,108,111,115	0
2	GOL	H	602	6/6	0.92	0.21	80,83,86,88	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.

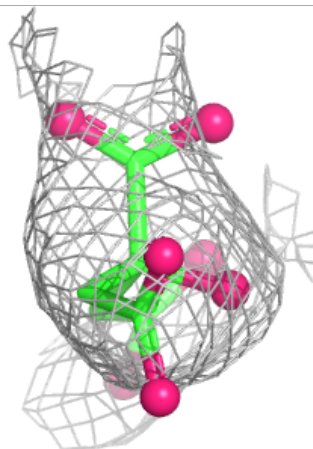
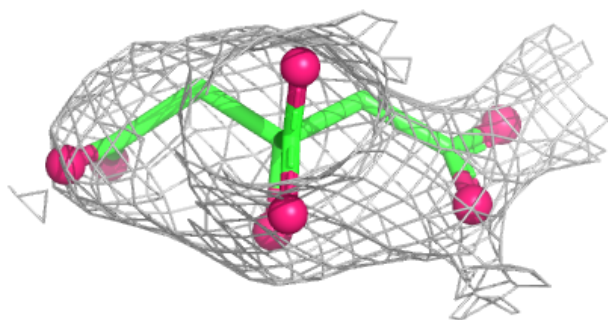
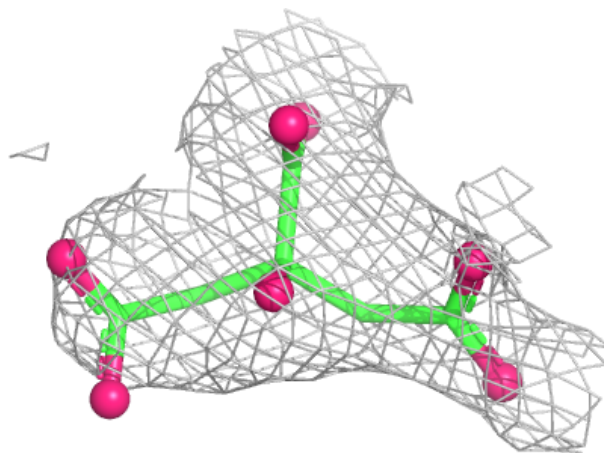
**Electron density around CIT D 601:**

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



**Electron density around CIT H 601:**

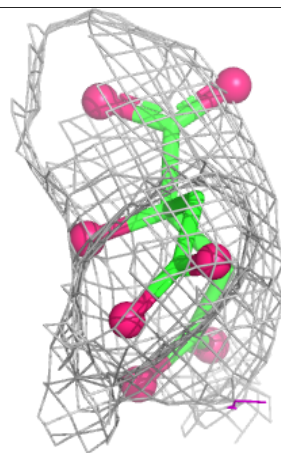
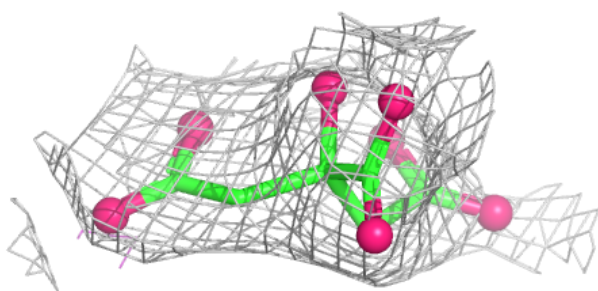
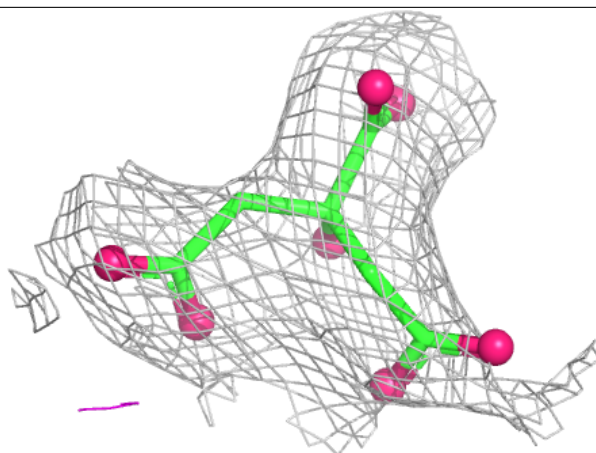
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



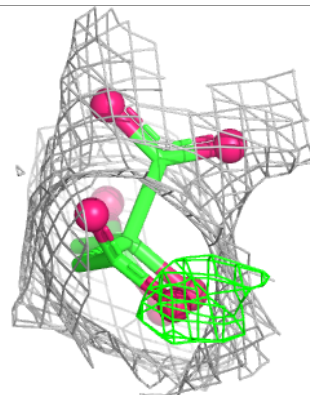
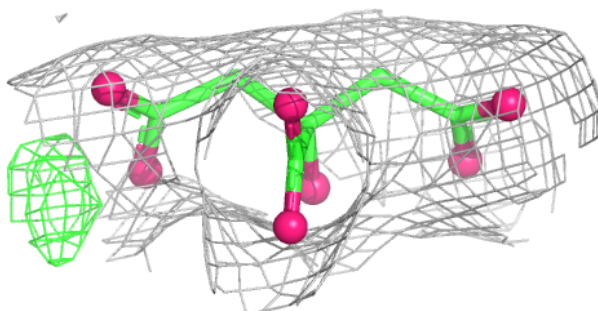
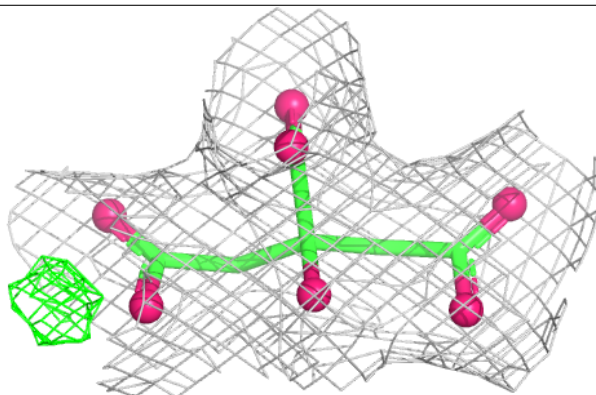


**Electron density around CIT F 601:**

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

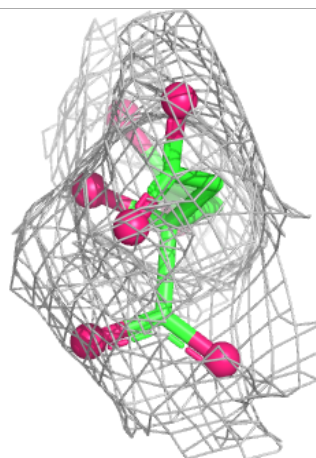
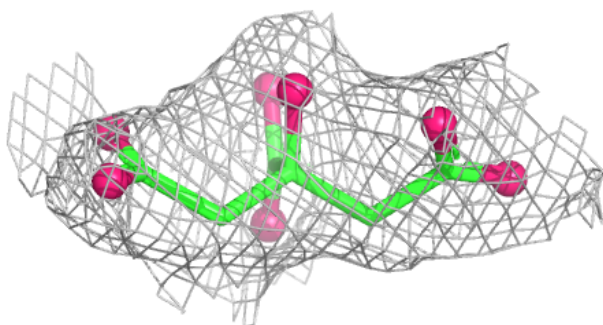
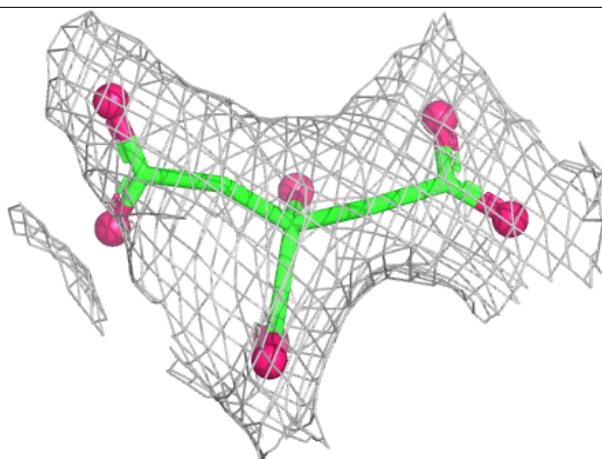
**Electron density around CIT C 601:**

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



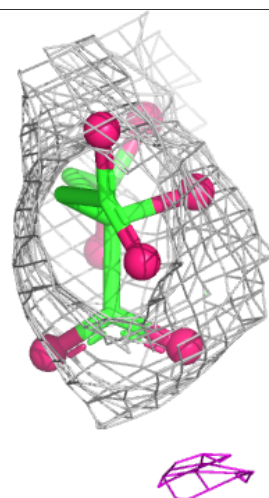
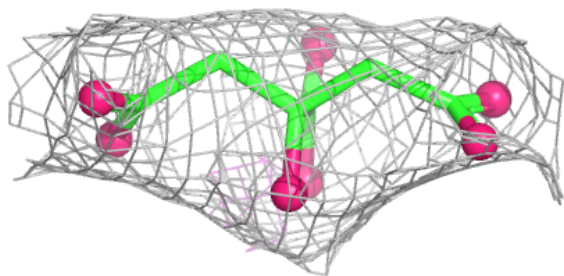
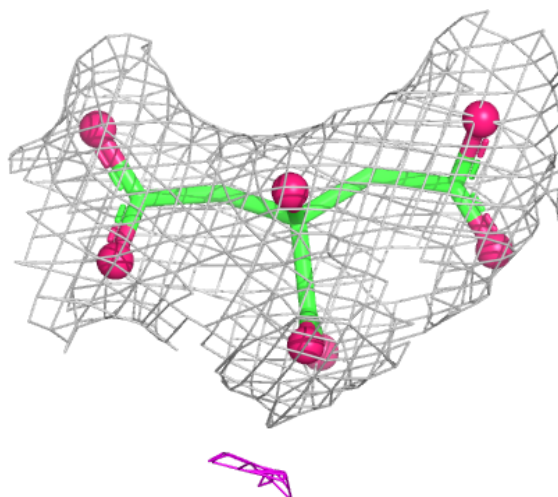
**Electron density around CIT B 601:**

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



**Electron density around CIT E 601:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.