



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 08:13 PM JST

PDB ID : 7F6E  
Title : Crystal structure of metal-citrate-binding protein (MctA) of ABC transporter endogenously bound to Mg<sup>2+</sup>-citrate complex (Form I)  
Authors : Kanaujia, S.P.; Mandal, S.K.; Gogoi, P.  
Deposited on : 2021-06-25  
Resolution : 1.77 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](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

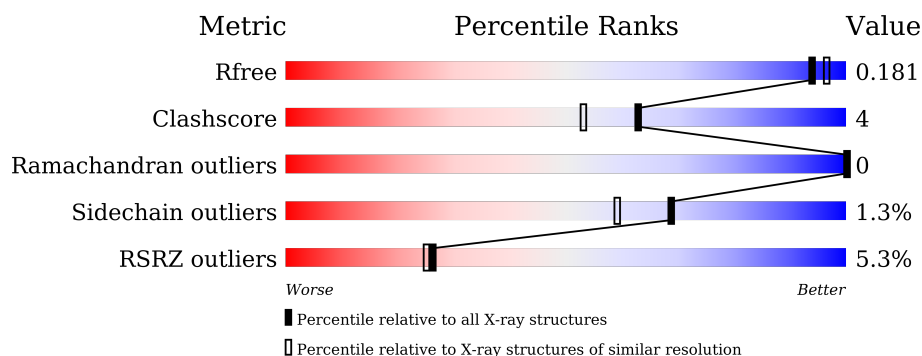
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	342	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>89%</span> <span>10%</span> <span>.</span> </div> </div>
1	B	342	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>2%</span> <span>88%</span> <span>10%</span> <span>.</span> </div> </div>
1	C	342	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>13%</span> <span>91%</span> <span>6%</span> <span>..</span> </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
5	CO2	A	407	-	-	X	-
6	GOL	B	411	-	-	X	-
7	EDO	B	417	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8990 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 Iron ABC transporter, periplasmic iron-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	7	0
			2720	1744	474	496	6			
1	B	341	Total	C	N	O	S	0	7	0
			2727	1749	472	500	6			
1	C	336	Total	C	N	O	S	0	0	0
			2648	1695	461	488	4			

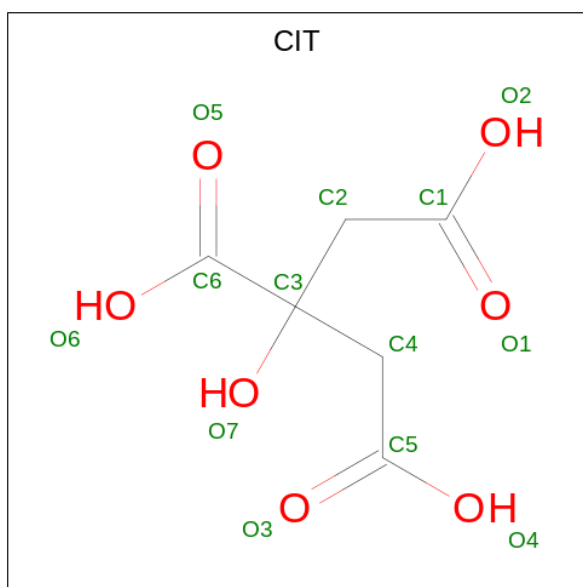
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q53VZ2
A	0	MET	-	expression tag	UNP Q53VZ2
B	-1	MET	-	initiating methionine	UNP Q53VZ2
B	0	MET	-	expression tag	UNP Q53VZ2
C	-1	MET	-	initiating methionine	UNP Q53VZ2
C	0	MET	-	expression tag	UNP Q53VZ2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).

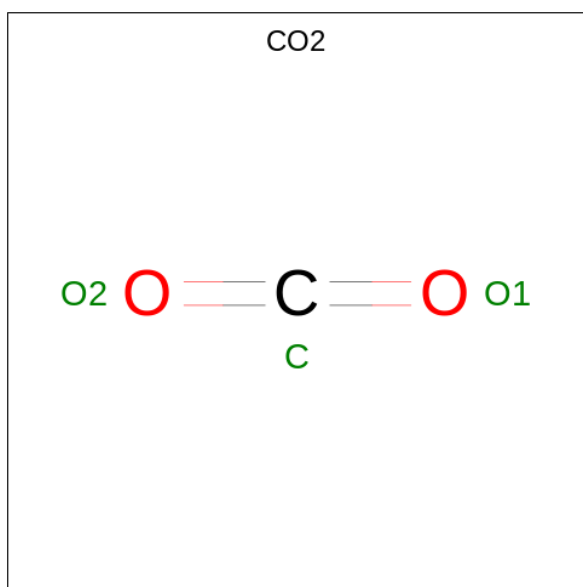


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Cl	0	0
			4	4		
4	B	4	Total	Cl	0	0
			4	4		

- Molecule 5 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO<sub>2</sub>).



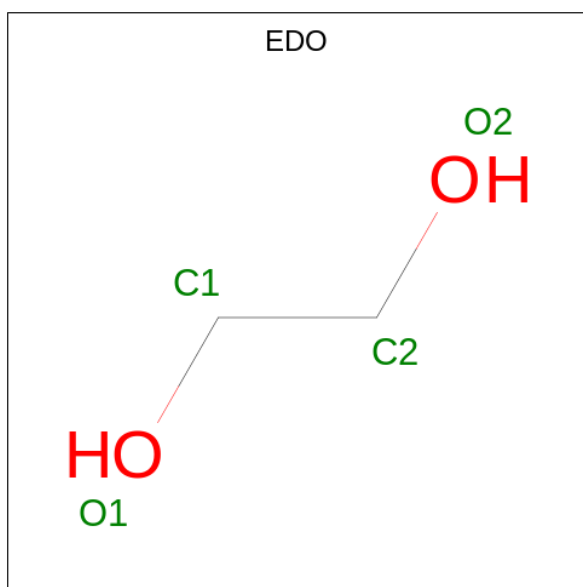
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).

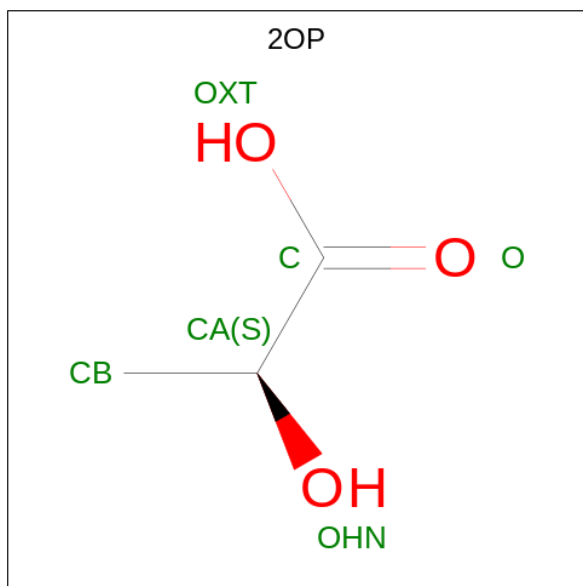


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total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

- Molecule 8 is (2S)-2-HYDROXYPROPANOIC ACID (three-letter code: 2OP) (formula:

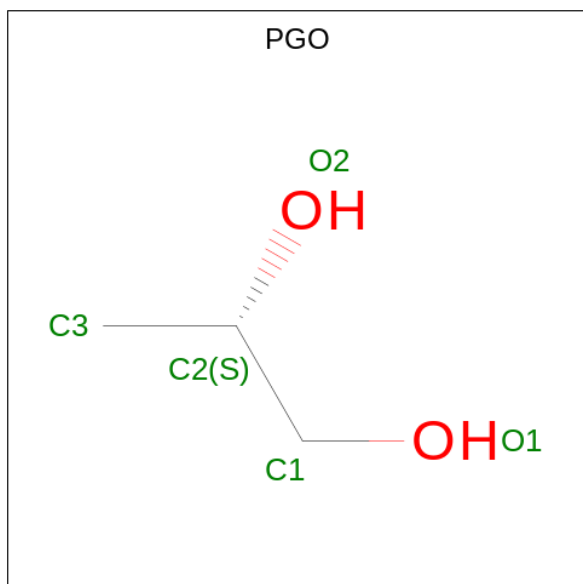


C<sub>3</sub>H<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			5	3	2		

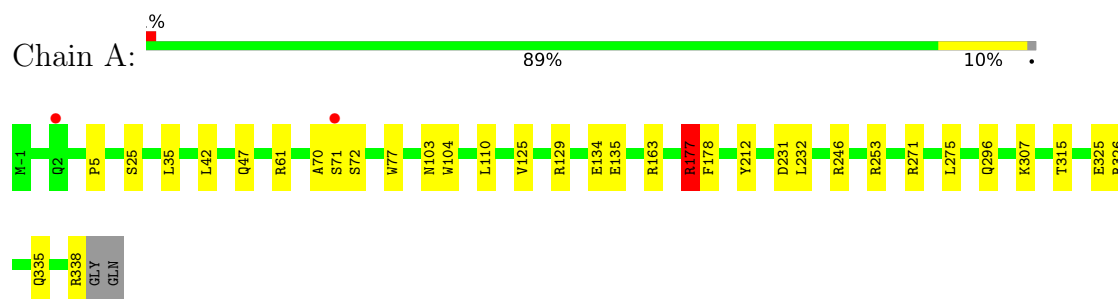
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	284	Total 284	O 284	0	0
10	B	297	Total 297	O 297	0	0
10	C	135	Total 135	O 135	0	0

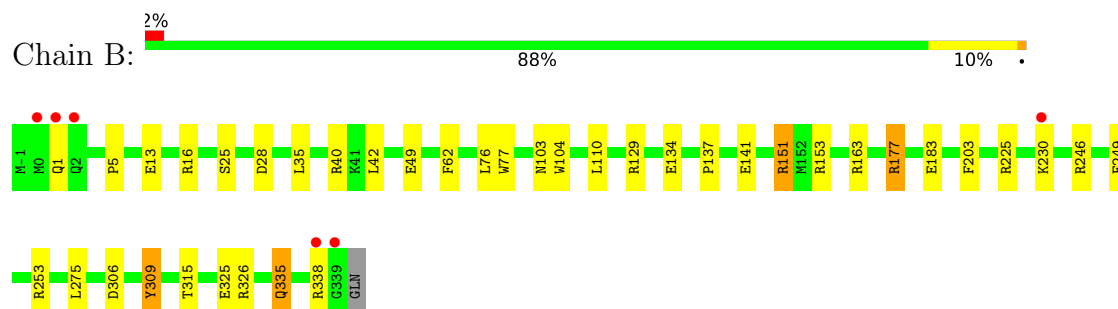
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

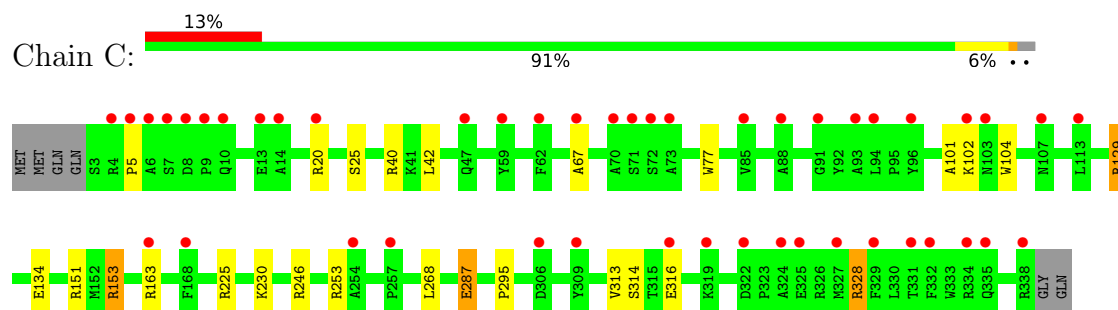
- Molecule 1: Iron ABC transporter, periplasmic iron-binding protein



- Molecule 1: Iron ABC transporter, periplasmic iron-binding protein



- Molecule 1: Iron ABC transporter, periplasmic iron-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.27Å 144.25Å 79.15Å 90.00° 100.16° 90.00°	Depositor
Resolution (Å)	52.98 – 1.77 52.93 – 1.77	Depositor EDS
% Data completeness (in resolution range)	95.6 (52.98-1.77) 95.6 (52.93-1.77)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.137 , 0.172 0.151 , 0.181	Depositor DCC
$R_{free}$ test set	4480 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.4	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8990	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: CO2, CL, GOL, PGO, EDO, CIT, MG, 2OP

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	0.93	2/2800 (0.1%)	1.04	11/3795 (0.3%)
1	B	0.91	2/2810 (0.1%)	1.01	13/3808 (0.3%)
1	C	0.80	0/2707	0.94	12/3672 (0.3%)
All	All	0.88	4/8317 (0.0%)	1.00	36/11275 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	GLU	CD-OE2	-8.90	1.15	1.25
1	A	135	GLU	CD-OE1	-7.75	1.17	1.25
1	B	325	GLU	CD-OE2	-6.31	1.18	1.25
1	B	49	GLU	CD-OE1	5.66	1.31	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	ARG	NE-CZ-NH2	-12.23	114.19	120.30
1	A	253	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	177[A]	ARG	NE-CZ-NH2	8.62	124.61	120.30
1	A	177[B]	ARG	NE-CZ-NH2	8.62	124.61	120.30
1	A	246	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	B	253	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	253	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	163	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	163	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	225	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	C	163	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	B	253	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	40	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	B	163	ARG	NE-CZ-NH1	6.76	123.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	246	ARG	CG-CD-NE	-6.69	97.76	111.80
1	B	163	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	C	328	ARG	CG-CD-NE	-6.60	97.93	111.80
1	B	309	TYR	CB-CG-CD2	6.51	124.91	121.00
1	B	151	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	C	253	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	177[A]	ARG	CB-CG-CD	5.78	126.63	111.60
1	A	177[B]	ARG	CB-CG-CD	5.78	126.63	111.60
1	C	129	ARG	CG-CD-NE	-5.67	99.90	111.80
1	C	225	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	C	151	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	C	246	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	246	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	153	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	212	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	C	129	ARG	NH1-CZ-NH2	5.25	125.17	119.40
1	A	246	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	20	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	246	ARG	CG-CD-NE	-5.06	101.17	111.80
1	C	153	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	335[A]	GLN	CB-CG-CD	5.04	124.69	111.60
1	B	335[B]	GLN	CB-CG-CD	5.04	124.69	111.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2720	0	2755	26	0
1	B	2727	0	2760	28	0
1	C	2648	0	2650	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	5	0	0
3	C	13	0	5	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	6	0	0	3	0
5	B	12	0	0	0	0
6	A	18	0	24	0	0
6	B	12	0	16	4	0
6	C	12	0	16	0	0
7	A	28	0	41	4	0
7	B	24	0	36	9	0
8	A	6	0	5	1	0
8	B	6	0	5	1	0
9	B	5	0	8	2	0
10	A	284	0	0	6	0
10	B	297	0	0	11	0
10	C	135	0	0	3	0
All	All	8990	0	8331	71	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (71) 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:307:LYS:NZ	10:A:501:HOH:O	1.85	1.08
1:B:13:GLU:OE2	1:B:16:ARG:NH1	1.97	0.97
1:A:296:GLN:HG2	5:A:407:CO2:O1	1.75	0.86
1:C:40:ARG:NH2	10:C:501:HOH:O	2.15	0.80
1:A:125[B]:VAL:CG1	1:A:232:LEU:HD11	2.12	0.79
1:B:103:ASN:HB3	10:B:744:HOH:O	1.83	0.78
1:B:203:PHE:HD2	6:B:411:GOL:H32	1.55	0.72
1:B:183:GLU:OE1	10:B:501:HOH:O	2.07	0.71
1:A:103[B]:ASN:ND2	10:A:505:HOH:O	2.24	0.71
7:A:416:EDO:H22	1:C:67:ALA:HB1	1.73	0.69
1:B:103:ASN:ND2	10:B:504:HOH:O	2.25	0.69
1:A:110[B]:LEU:HD11	1:A:315:THR:HG23	1.76	0.67
1:A:70:ALA:O	10:A:502:HOH:O	2.14	0.66
1:B:110[B]:LEU:HD11	1:B:315:THR:HG23	1.78	0.65
1:B:137:PRO:HB3	7:B:413:EDO:H11	1.81	0.63
1:B:203:PHE:CD2	6:B:411:GOL:H32	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLU:CD	1:B:16:ARG:HH12	2.05	0.61
5:A:407:CO2:O2	10:A:503:HOH:O	2.17	0.59
1:B:35:LEU:HD23	1:B:275[A]:LEU:HD22	1.85	0.58
1:C:314:SER:OG	1:C:316:GLU:HG2	2.04	0.58
1:A:72:SER:H	7:A:414:EDO:C1	2.17	0.57
1:C:5:PRO:HD2	1:C:42:LEU:HD21	1.85	0.57
1:B:177[A]:ARG:HD3	9:B:419:PGO:O1	2.05	0.56
1:A:5:PRO:HD2	1:A:42[A]:LEU:HD21	1.87	0.56
1:C:313:VAL:O	10:C:502:HOH:O	2.18	0.56
1:A:177[A]:ARG:HD2	1:A:178:PHE:CZ	2.40	0.56
1:A:315:THR:HG21	1:B:110[B]:LEU:HD12	1.85	0.56
1:A:42[B]:LEU:HD21	1:A:271:ARG:NH1	2.21	0.56
1:C:129:ARG:O	1:C:129:ARG:HG2	2.05	0.56
1:A:61:ARG:NH1	10:A:508:HOH:O	2.38	0.55
1:A:134:GLU:H	1:A:134:GLU:CD	2.09	0.55
1:B:134:GLU:H	1:B:134:GLU:CD	2.10	0.54
1:B:1:GLN:H	1:B:1:GLN:CD	2.11	0.54
7:B:417:EDO:C1	10:B:678:HOH:O	2.55	0.54
1:B:76[B]:LEU:HD12	1:B:249:PHE:CZ	2.43	0.53
1:B:28:ASP:OD2	6:B:411:GOL:H12	2.09	0.53
1:A:47:GLN:OE1	10:A:504:HOH:O	2.18	0.52
1:C:134:GLU:H	1:C:134:GLU:CD	2.13	0.51
7:B:417:EDO:H12	10:B:678:HOH:O	2.11	0.51
1:B:5:PRO:HD2	1:B:42:LEU:HD21	1.93	0.51
1:A:5:PRO:CD	1:A:42[A]:LEU:HD21	2.41	0.50
1:A:129:ARG:NH1	1:A:231:ASP:OD2	2.35	0.49
1:A:296:GLN:CG	5:A:407:CO2:O1	2.55	0.49
1:A:125[B]:VAL:HG12	1:A:232:LEU:HD11	1.93	0.49
1:B:177[A]:ARG:HD2	1:B:309:TYR:CG	2.48	0.49
7:B:417:EDO:C2	10:B:678:HOH:O	2.60	0.49
1:A:71:SER:HA	7:A:414:EDO:H22	1.96	0.47
1:A:103[B]:ASN:OD1	8:A:419:2OP:OXT	2.32	0.47
1:B:137:PRO:CB	7:B:413:EDO:H11	2.42	0.47
1:A:129:ARG:HD3	1:A:231:ASP:OD2	2.16	0.46
1:B:129:ARG:NH1	10:B:507:HOH:O	2.33	0.46
1:B:141:GLU:OE2	1:C:328:ARG:NH2	2.33	0.45
1:B:335[A]:GLN:HG3	10:B:618:HOH:O	2.16	0.45
1:C:287:GLU:HG3	1:C:295:PRO:HB2	1.99	0.45
7:B:414:EDO:C2	10:B:515:HOH:O	2.65	0.44
1:C:153:ARG:HD3	10:C:519:HOH:O	2.18	0.44
1:B:151:ARG:HD2	7:B:418:EDO:H11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLN:O	1:A:338:ARG:HG2	2.19	0.43
1:A:35:LEU:HD23	1:A:275:LEU:HD22	1.99	0.43
7:B:414:EDO:H22	10:B:515:HOH:O	2.18	0.43
1:B:306:ASP:O	9:B:419:PGO:H2	2.17	0.43
1:C:25:SER:HA	1:C:77:TRP:O	2.19	0.43
1:B:103:ASN:OD1	8:B:420:2OP:OXT	2.37	0.42
1:A:326:ARG:NH2	7:A:412:EDO:O2	2.53	0.42
1:B:28:ASP:OD2	6:B:411:GOL:C1	2.68	0.42
1:B:25:SER:HA	1:B:77:TRP:O	2.19	0.42
1:A:25:SER:HA	1:A:77:TRP:O	2.20	0.41
1:A:177[A]:ARG:HD2	1:A:178:PHE:CE1	2.55	0.41
7:B:417:EDO:H21	10:B:678:HOH:O	2.18	0.41
1:C:101:ALA:HB2	1:C:268:LEU:HD13	2.02	0.40
1:B:62:PHE:CD2	1:B:76[B]:LEU:HD11	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/342 (101%)	340 (99%)	5 (1%)	0	100	100
1	B	347/342 (102%)	341 (98%)	6 (2%)	0	100	100
1	C	334/342 (98%)	330 (99%)	4 (1%)	0	100	100
All	All	1026/1026 (100%)	1011 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	280/274 (102%)	277 (99%)	3 (1%)	73	65
1	B	281/274 (103%)	275 (98%)	6 (2%)	53	38
1	C	269/274 (98%)	265 (98%)	4 (2%)	65	53
All	All	830/822 (101%)	817 (98%)	13 (2%)	69	51

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	TRP
1	A	177[A]	ARG
1	A	177[B]	ARG
1	B	104	TRP
1	B	177[A]	ARG
1	B	177[B]	ARG
1	B	230	LYS
1	B	326	ARG
1	B	338	ARG
1	C	102	LYS
1	C	104	TRP
1	C	230	LYS
1	C	287	GLU

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 43 ligands modelled in this entry, 11 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	EDO	A	418	-	3,3,3	0.11	0	2,2,2	0.15	0
7	EDO	B	417	-	3,3,3	0.47	0	2,2,2	0.57	0
3	CIT	A	402	2	3,12,12	0.66	0	3,17,17	0.40	0
6	GOL	A	409	-	5,5,5	0.18	0	5,5,5	0.39	0
7	EDO	B	418	-	3,3,3	0.10	0	2,2,2	0.05	0
5	CO2	B	409	-	2,2,2	0.03	0	1,1,1	0.84	0
7	EDO	B	416	-	3,3,3	0.15	0	2,2,2	0.42	0
3	CIT	B	402	2	3,12,12	1.00	0	3,17,17	0.59	0
5	CO2	B	410	-	2,2,2	0.11	0	1,1,1	0.85	0
6	GOL	C	403	-	5,5,5	0.13	0	5,5,5	0.24	0
3	CIT	C	402	2	3,12,12	0.69	0	3,17,17	0.78	0
7	EDO	A	414	-	3,3,3	0.53	0	2,2,2	0.19	0
8	2OP	B	420	-	2,5,5	0.27	0	3,6,6	0.61	0
7	EDO	B	414	-	3,3,3	0.66	0	2,2,2	0.51	0
7	EDO	B	413	-	3,3,3	0.55	0	2,2,2	0.06	0
5	CO2	B	408	-	2,2,2	0.20	0	1,1,1	0.73	0
6	GOL	B	412	-	5,5,5	0.21	0	5,5,5	0.63	0
6	GOL	A	411	-	5,5,5	0.25	0	5,5,5	0.48	0
7	EDO	A	415	-	3,3,3	1.09	0	2,2,2	0.43	0
8	2OP	A	419	-	2,5,5	0.21	0	3,6,6	0.48	0
6	GOL	A	410	-	5,5,5	0.07	0	5,5,5	0.13	0
7	EDO	A	412	-	3,3,3	0.21	0	2,2,2	0.06	0
6	GOL	C	404	-	5,5,5	0.14	0	5,5,5	0.25	0
5	CO2	A	407	-	2,2,2	0.09	0	1,1,1	0.90	0
7	EDO	A	417	-	3,3,3	0.07	0	2,2,2	0.11	0
9	PGO	B	419	-	3,4,4	0.09	0	1,4,4	0.42	0
7	EDO	B	415	-	3,3,3	0.37	0	2,2,2	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	A	416	-	3,3,3	0.08	0	2,2,2	0.19	0
7	EDO	A	413	-	3,3,3	0.25	0	2,2,2	0.33	0
5	CO2	A	408	-	2,2,2	0.26	0	1,1,1	0.79	0
6	GOL	B	411	-	5,5,5	0.14	0	5,5,5	0.43	0
5	CO2	B	407	-	2,2,2	0.18	0	1,1,1	0.75	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
7	EDO	A	418	-	-	1/1/1/1	-
7	EDO	B	417	-	-	1/1/1/1	-
3	CIT	A	402	2	-	0/6/16/16	-
6	GOL	A	409	-	-	2/4/4/4	-
7	EDO	B	418	-	-	1/1/1/1	-
7	EDO	B	416	-	-	1/1/1/1	-
3	CIT	B	402	2	-	0/6/16/16	-
6	GOL	C	403	-	-	0/4/4/4	-
3	CIT	C	402	2	-	0/6/16/16	-
7	EDO	A	414	-	-	1/1/1/1	-
8	2OP	B	420	-	-	0/0/4/4	-
7	EDO	B	414	-	-	0/1/1/1	-
7	EDO	B	413	-	-	1/1/1/1	-
6	GOL	B	412	-	-	0/4/4/4	-
6	GOL	A	411	-	-	2/4/4/4	-
7	EDO	A	415	-	-	1/1/1/1	-
8	2OP	A	419	-	-	0/0/4/4	-
6	GOL	A	410	-	-	0/4/4/4	-
7	EDO	A	412	-	-	1/1/1/1	-
6	GOL	C	404	-	-	1/4/4/4	-
7	EDO	A	417	-	-	1/1/1/1	-
9	PGO	B	419	-	-	2/2/2/2	-
7	EDO	B	415	-	-	1/1/1/1	-
7	EDO	A	416	-	-	1/1/1/1	-
7	EDO	A	413	-	-	1/1/1/1	-
6	GOL	B	411	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	409	GOL	O1-C1-C2-C3
6	B	411	GOL	C1-C2-C3-O3
9	B	419	PGO	O1-C1-C2-C3
7	A	418	EDO	O1-C1-C2-O2
6	A	411	GOL	O1-C1-C2-C3
6	A	409	GOL	O1-C1-C2-O2
6	B	411	GOL	O2-C2-C3-O3
7	A	413	EDO	O1-C1-C2-O2
7	A	415	EDO	O1-C1-C2-O2
7	A	416	EDO	O1-C1-C2-O2
7	A	417	EDO	O1-C1-C2-O2
6	C	404	GOL	O1-C1-C2-C3
9	B	419	PGO	O1-C1-C2-O2
7	B	413	EDO	O1-C1-C2-O2
7	B	415	EDO	O1-C1-C2-O2
7	B	416	EDO	O1-C1-C2-O2
6	A	411	GOL	O1-C1-C2-O2
7	A	412	EDO	O1-C1-C2-O2
7	A	414	EDO	O1-C1-C2-O2
7	B	417	EDO	O1-C1-C2-O2
7	B	418	EDO	O1-C1-C2-O2

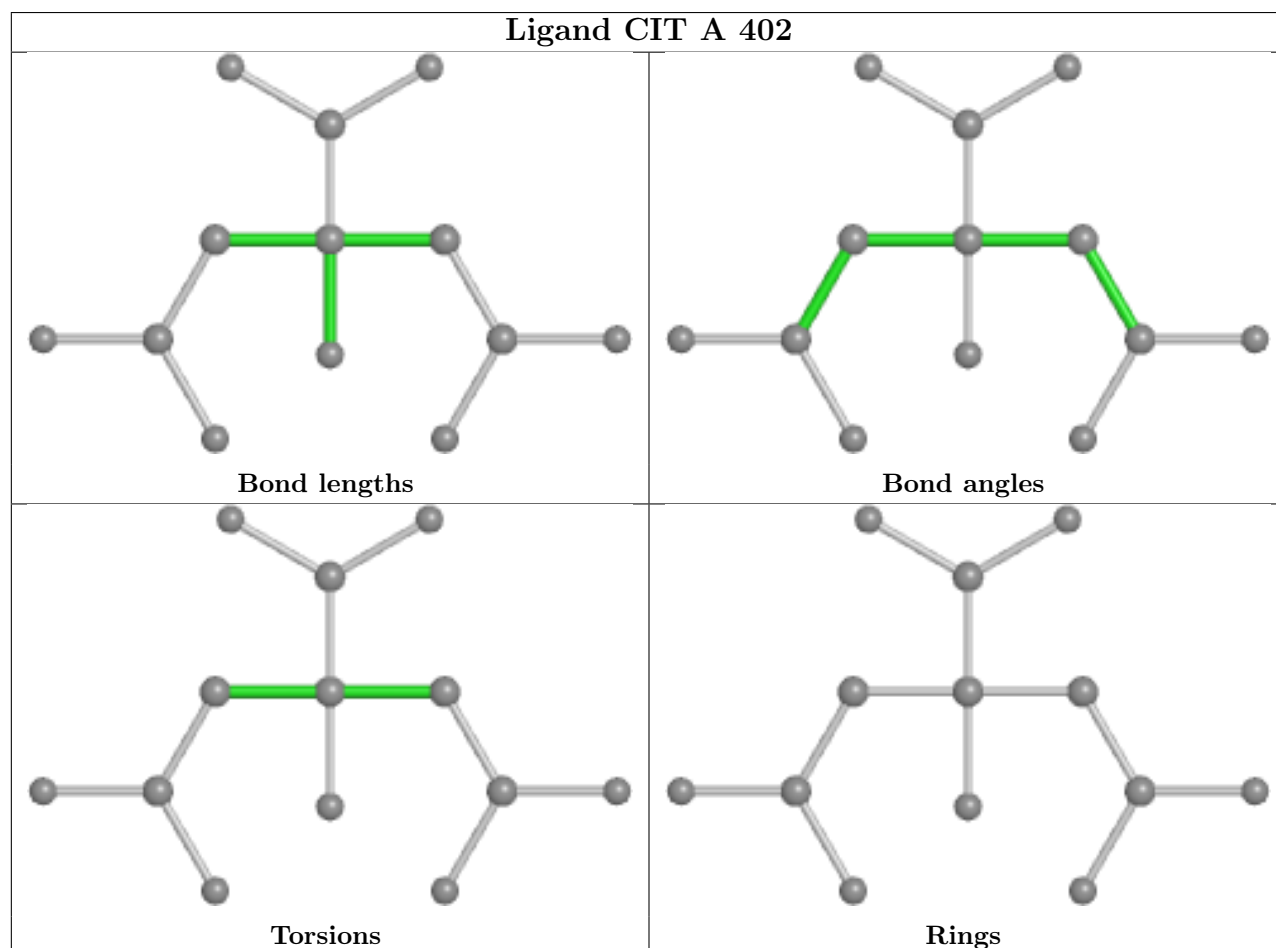
There are no ring outliers.

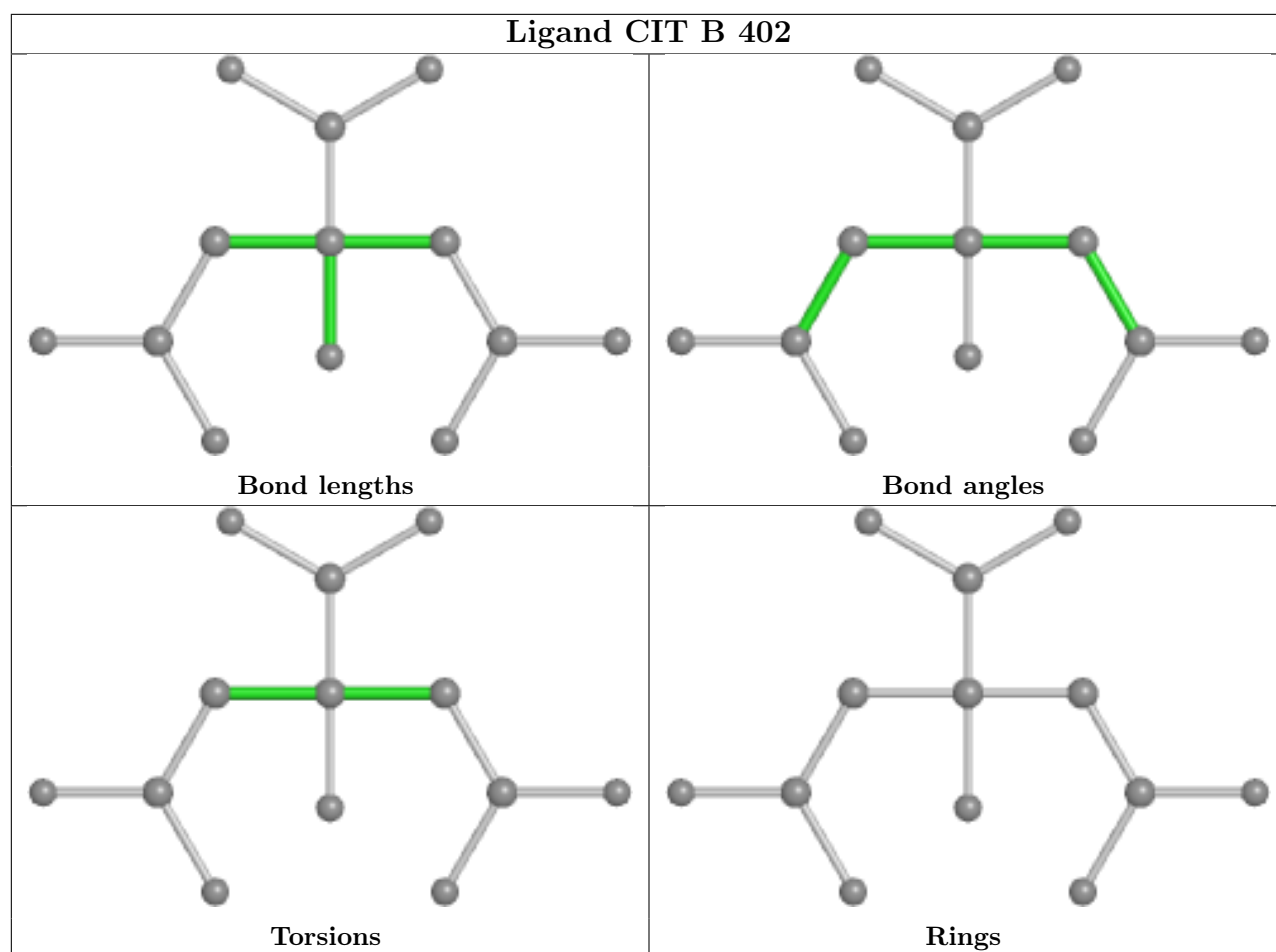
12 monomers are involved in 24 short contacts:

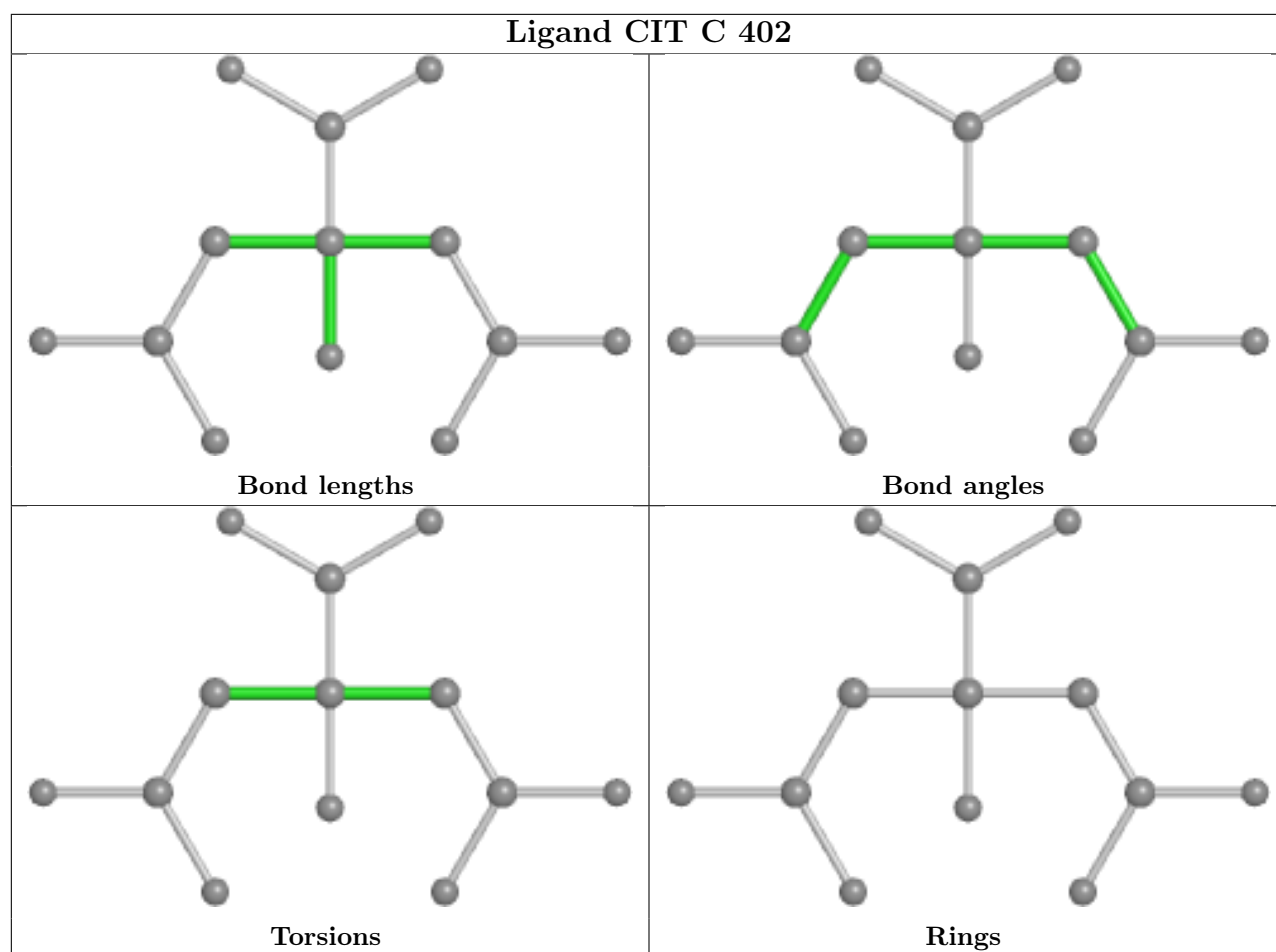
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	417	EDO	4	0
7	B	418	EDO	1	0
7	A	414	EDO	2	0
8	B	420	2OP	1	0
7	B	414	EDO	2	0
7	B	413	EDO	2	0
8	A	419	2OP	1	0
7	A	412	EDO	1	0
5	A	407	CO2	3	0
9	B	419	PGO	2	0
7	A	416	EDO	1	0
6	B	411	GOL	4	0

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

### 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<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	340/342 (99%)	-0.10	2 (0%) 89 89	9, 15, 30, 50	0
1	B	341/342 (99%)	-0.25	6 (1%) 68 68	9, 16, 30, 53	0
1	C	336/342 (98%)	0.55	46 (13%) 3 2	17, 30, 55, 70	0
All	All	1017/1026 (99%)	0.06	54 (5%) 26 25	9, 19, 46, 70	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	71	SER	6.3
1	C	324	ALA	5.6
1	C	6	ALA	5.2
1	C	322	ASP	4.5
1	A	71	SER	3.4
1	B	1	GLN	3.2
1	C	9	PRO	3.1
1	C	72	SER	3.1
1	C	20	ARG	3.0
1	C	7	SER	3.0
1	C	94	LEU	3.0
1	C	59	TYR	2.9
1	C	4	ARG	2.9
1	C	334	ARG	2.9
1	C	107	ASN	2.7
1	C	91	GLY	2.7
1	C	103	ASN	2.7
1	C	5	PRO	2.7
1	C	309	TYR	2.6
1	B	339	GLY	2.6
1	B	2	GLN	2.6
1	A	2	GLN	2.6
1	C	47	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	257	PRO	2.6
1	C	329	PHE	2.5
1	C	335	GLN	2.5
1	C	85	VAL	2.5
1	C	319	LYS	2.4
1	C	73	ALA	2.4
1	C	254	ALA	2.4
1	C	113	LEU	2.3
1	C	331	THR	2.3
1	C	332	PHE	2.3
1	C	67	ALA	2.2
1	C	88	ALA	2.2
1	B	230	LYS	2.2
1	C	96	TYR	2.2
1	B	0	MET	2.2
1	C	102	LYS	2.2
1	C	70	ALA	2.2
1	C	93	ALA	2.2
1	C	163	ARG	2.2
1	C	306	ASP	2.2
1	C	13	GLU	2.1
1	C	327	MET	2.1
1	C	10	GLN	2.1
1	C	316	GLU	2.1
1	C	62	PHE	2.1
1	C	338	ARG	2.1
1	C	168	PHE	2.1
1	C	325	GLU	2.1
1	B	338	ARG	2.0
1	C	8	ASP	2.0
1	C	14	ALA	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

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
7	EDO	A	414	4/4	0.79	0.15	36,36,38,42	0
7	EDO	A	417	4/4	0.79	0.14	52,53,57,58	0
8	2OP	A	419	6/6	0.83	0.16	44,49,51,52	0
7	EDO	B	418	4/4	0.86	0.28	37,38,40,44	0
5	CO2	B	407	3/3	0.87	0.09	51,51,53,56	0
7	EDO	A	418	4/4	0.88	0.14	42,45,46,49	0
7	EDO	B	414	4/4	0.88	0.15	23,29,32,36	0
7	EDO	A	416	4/4	0.88	0.10	42,45,45,46	0
6	GOL	B	411	6/6	0.88	0.20	27,33,36,38	0
9	PGO	B	419	5/5	0.88	0.12	39,41,43,48	0
7	EDO	B	416	4/4	0.89	0.14	44,45,47,47	0
6	GOL	A	409	6/6	0.89	0.14	26,36,39,41	0
5	CO2	B	408	3/3	0.90	0.09	32,32,43,45	0
5	CO2	A	408	3/3	0.90	0.14	41,41,48,51	0
6	GOL	C	404	6/6	0.91	0.12	32,40,41,42	0
6	GOL	A	410	6/6	0.91	0.14	24,32,34,36	0
6	GOL	A	411	6/6	0.92	0.10	26,29,30,37	0
7	EDO	B	415	4/4	0.92	0.15	33,34,34,39	0
8	2OP	B	420	6/6	0.92	0.11	34,44,47,47	0
7	EDO	A	412	4/4	0.92	0.10	34,42,42,43	0
7	EDO	A	413	4/4	0.94	0.10	26,32,33,36	0
5	CO2	B	410	3/3	0.94	0.12	52,52,52,53	0
6	GOL	C	403	6/6	0.94	0.12	33,39,40,41	0
4	CL	A	403	1/1	0.95	0.06	29,29,29,29	0
3	CIT	C	402	13/13	0.95	0.11	21,22,25,26	0
5	CO2	B	409	3/3	0.96	0.18	31,31,34,38	0
5	CO2	A	407	3/3	0.96	0.14	35,35,40,43	0
7	EDO	B	413	4/4	0.96	0.23	33,35,37,39	0
7	EDO	B	417	4/4	0.96	0.10	22,22,27,28	0
6	GOL	B	412	6/6	0.97	0.08	23,25,25,26	0
4	CL	A	406	1/1	0.97	0.09	35,35,35,35	0
4	CL	B	406	1/1	0.97	0.09	35,35,35,35	0
7	EDO	A	415	4/4	0.97	0.14	21,22,25,26	0
3	CIT	A	402	13/13	0.98	0.09	11,12,14,14	0
4	CL	B	404	1/1	0.98	0.07	28,28,28,28	0
3	CIT	B	402	13/13	0.98	0.07	11,12,13,14	0
4	CL	A	404	1/1	0.98	0.05	27,27,27,27	0

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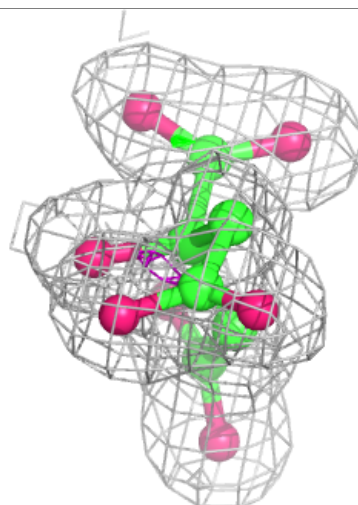
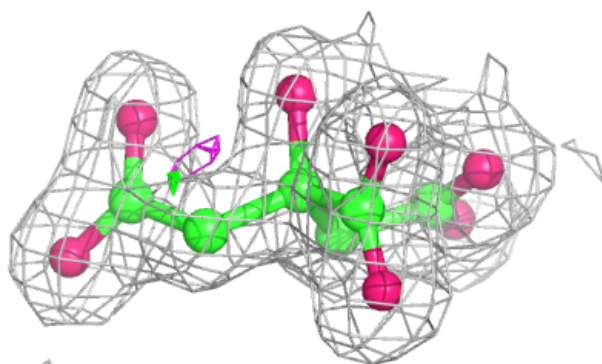
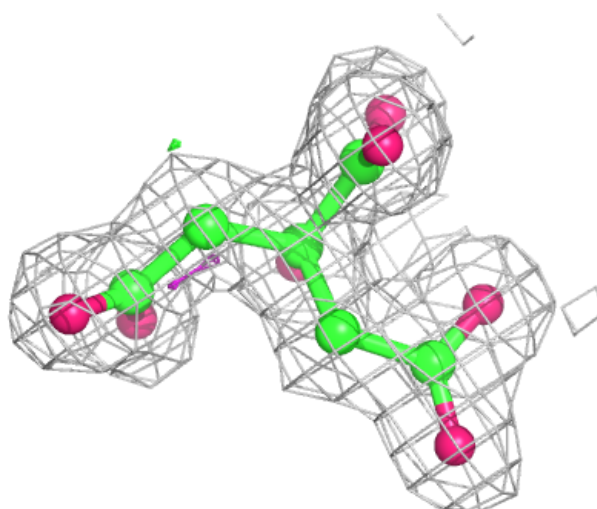
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	A	405	1/1	0.99	0.08	32,32,32,32	0
4	CL	B	405	1/1	0.99	0.05	31,31,31,31	0
2	MG	C	401	1/1	0.99	0.10	23,23,23,23	0
4	CL	B	403	1/1	0.99	0.05	28,28,28,28	0
2	MG	B	401	1/1	1.00	0.07	16,16,16,16	0
2	MG	A	401	1/1	1.00	0.06	14,14,14,14	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.

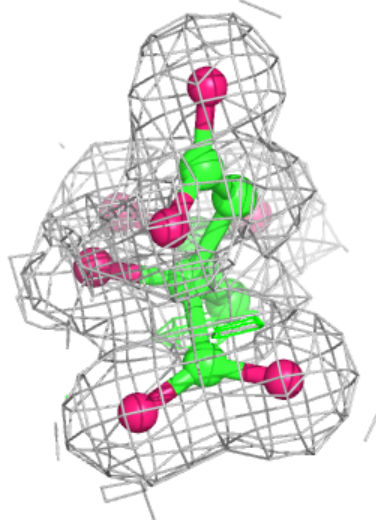
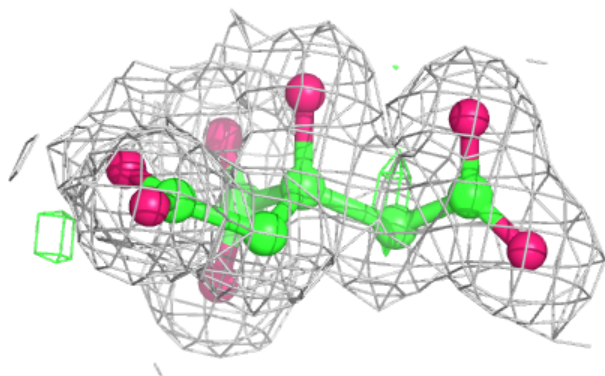
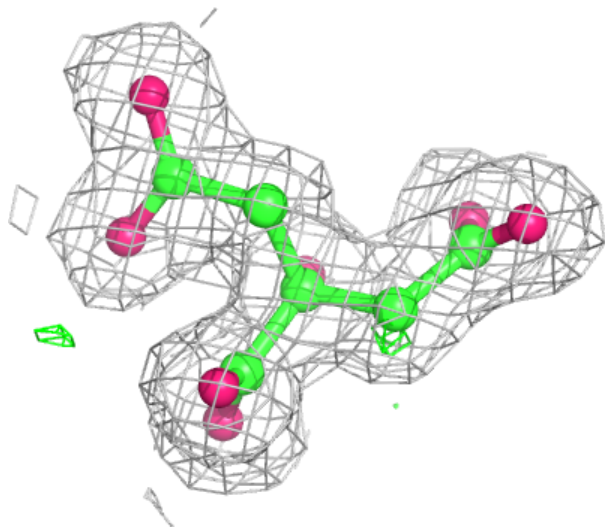
**Electron density around CIT C 402:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



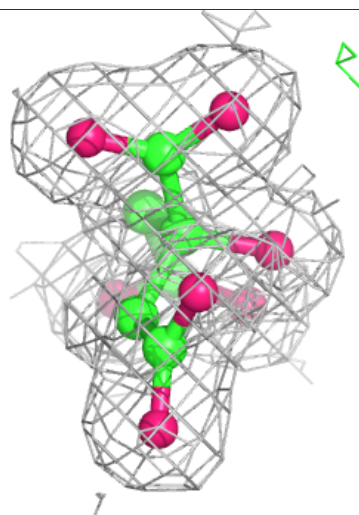
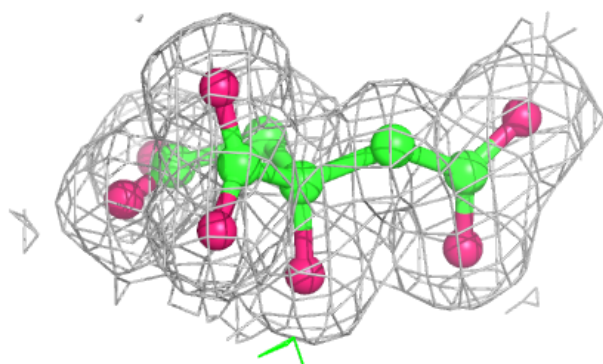
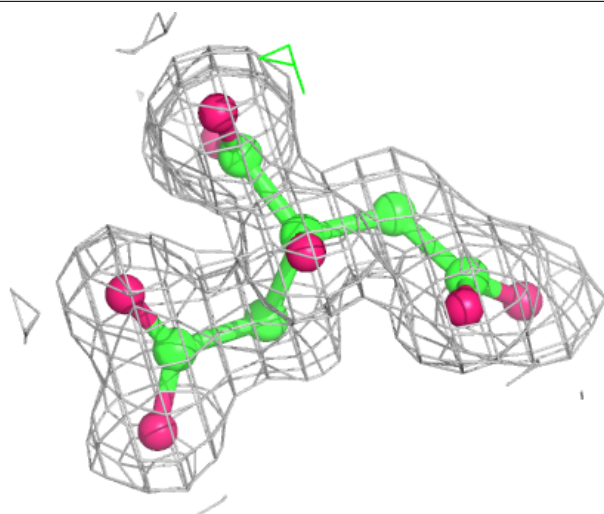
**Electron density around CIT A 402:**

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



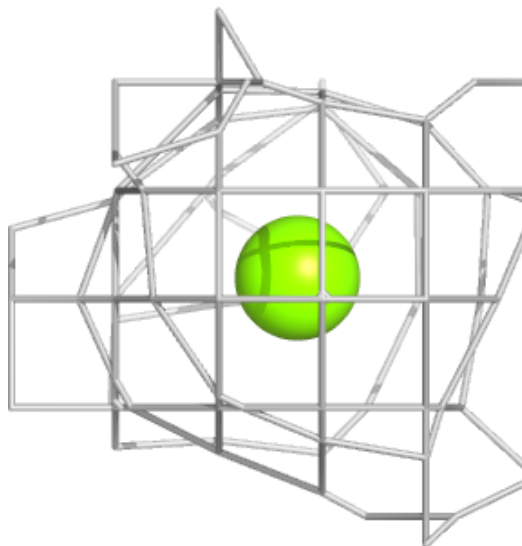
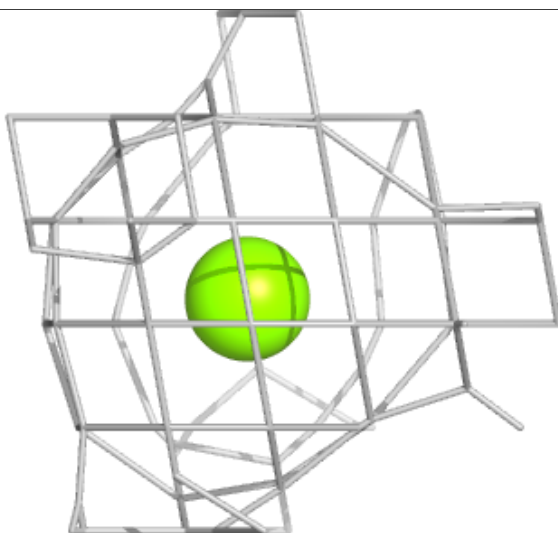
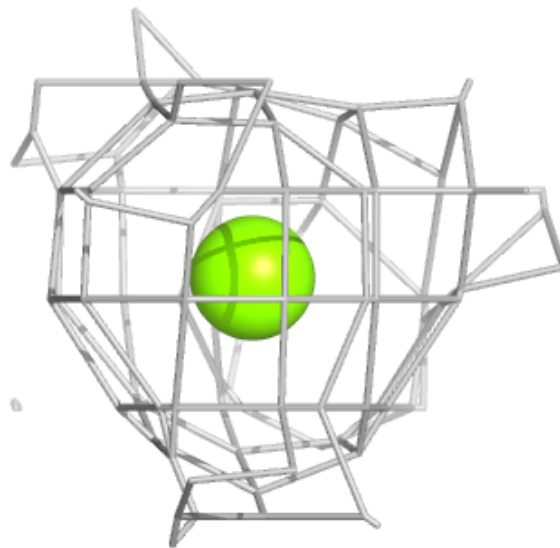
**Electron density around CIT B 402:**

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



**Electron density around MG C 401:**

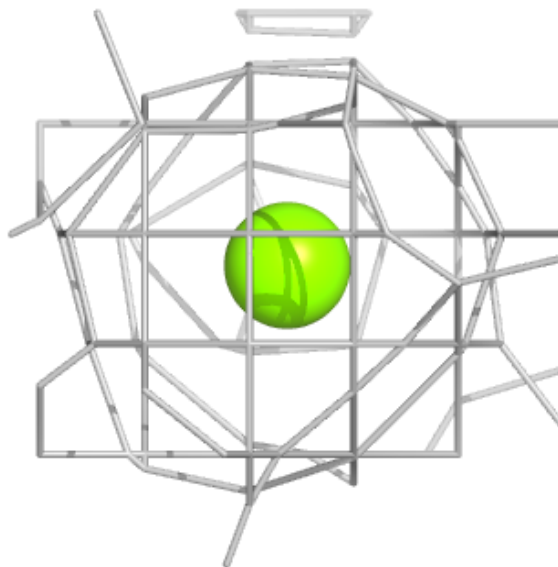
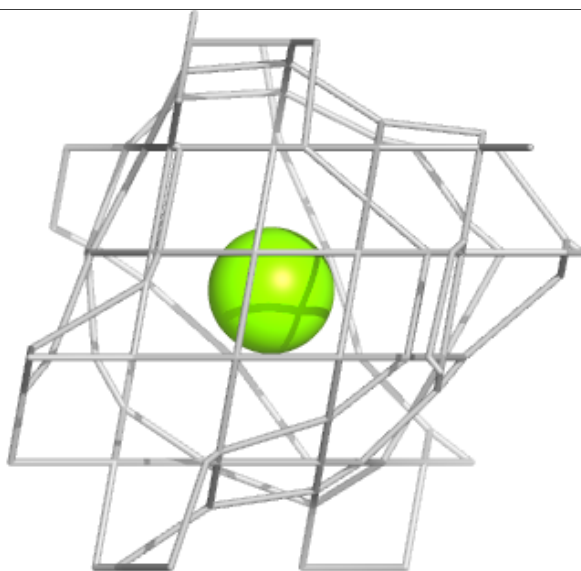
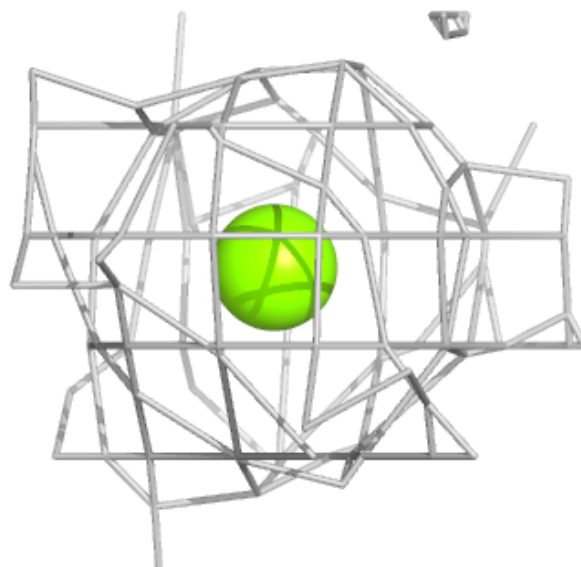
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG B 401:**

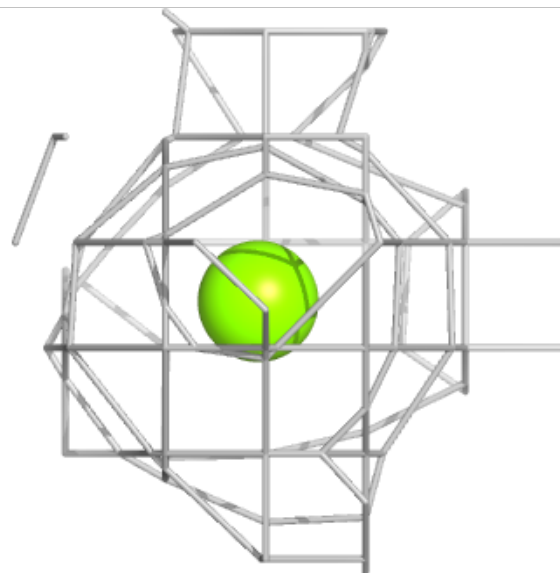
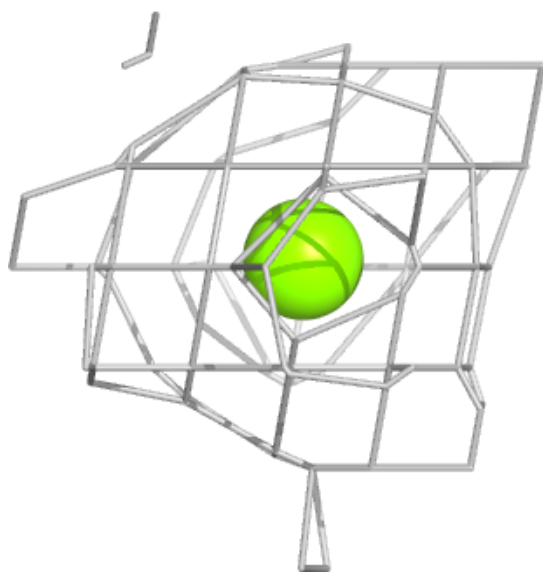
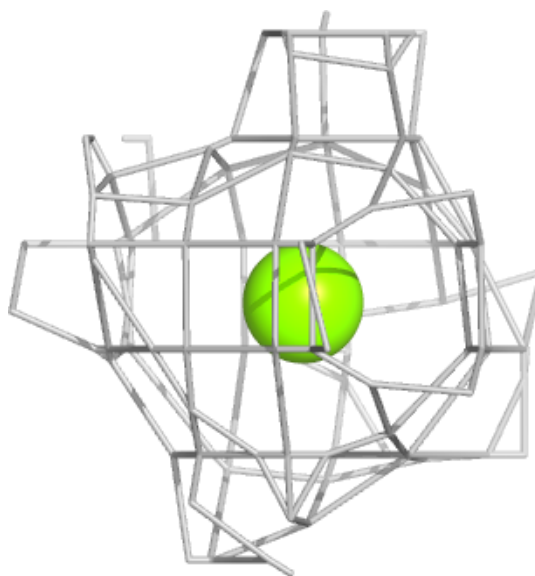
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG A 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.