



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:14 AM UTC

PDB ID : 7F6P / pdb_00007f6p
Title : Crystal structure of metal-citrate-binding mutant (D28A) protein (MctA) of ABC transporter endogenously bound to citrate
Authors : Kanaujia, S.P.; Mandal, S.K.
Deposited on : 2021-06-25
Resolution : 2.15 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

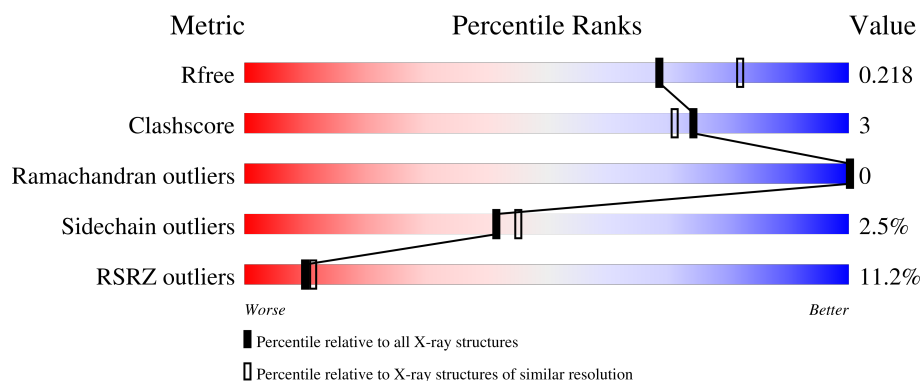
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	342	87% 9% . .
1	B	342	90% 6% . .
1	C	342	32% 89% 9% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8484 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	336	Total	C	N	O	S	0	2	0
			2661	1704	467	486	4			
1	B	336	Total	C	N	O	S	0	2	0
			2658	1704	464	486	4			
1	C	336	Total	C	N	O	S	0	0	0
			2645	1694	461	486	4			

There are 9 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
A	28	ALA	ASP	engineered mutation	UNP Q53VZ2
B	-1	MET	-	initiating methionine	UNP Q53VZ2
B	0	MET	-	expression tag	UNP Q53VZ2
B	28	ALA	ASP	engineered mutation	UNP Q53VZ2
C	-1	MET	-	initiating methionine	UNP Q53VZ2
C	0	MET	-	expression tag	UNP Q53VZ2
C	28	ALA	ASP	engineered mutation	UNP Q53VZ2

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



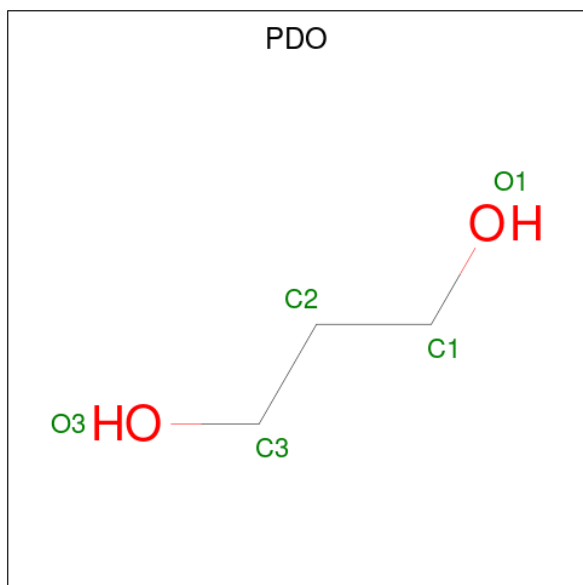
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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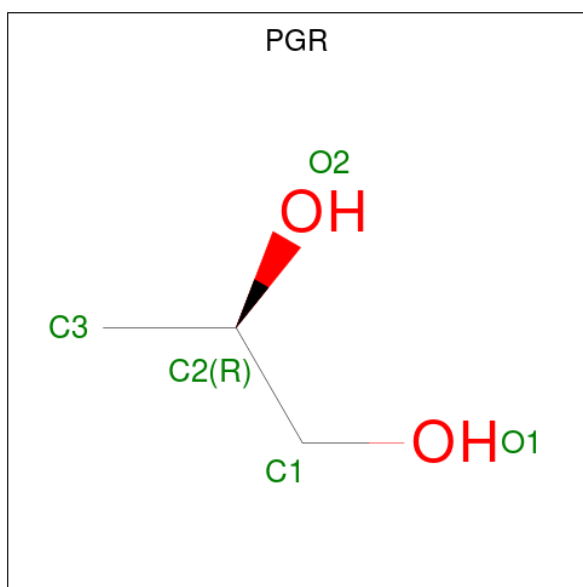
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,3-PROPANDIOL (CCD ID: PDO) (formula: $C_3H_8O_2$).



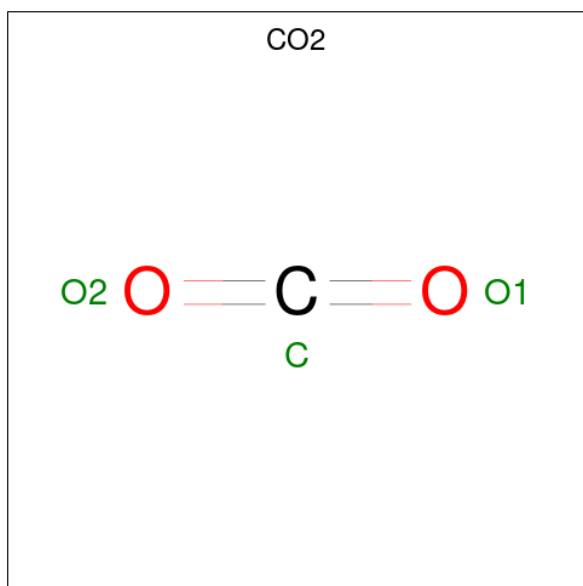
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 5 is R-1,2-PROPANEDIOL (CCD ID: PGR) (formula: $C_3H_8O_2$).



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

- Molecule 6 is CARBON DIOXIDE (CCD ID: CO2) (formula: CO₂).



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

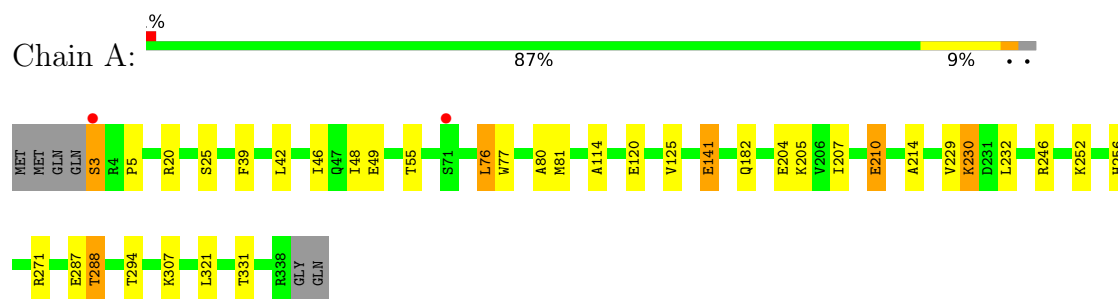
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	219	Total 219	O 219	0	0
7	B	217	Total 217	O 217	0	0
7	C	16	Total 16	O 16	0	0

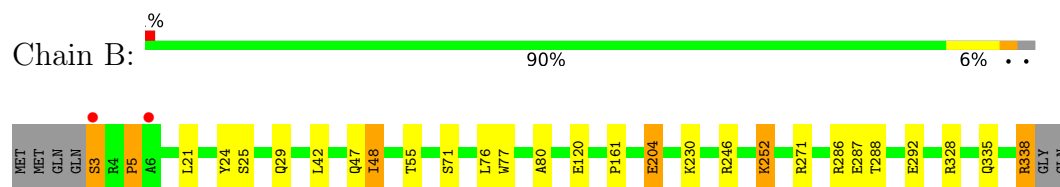
3 Residue-property plots [i](#)

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.

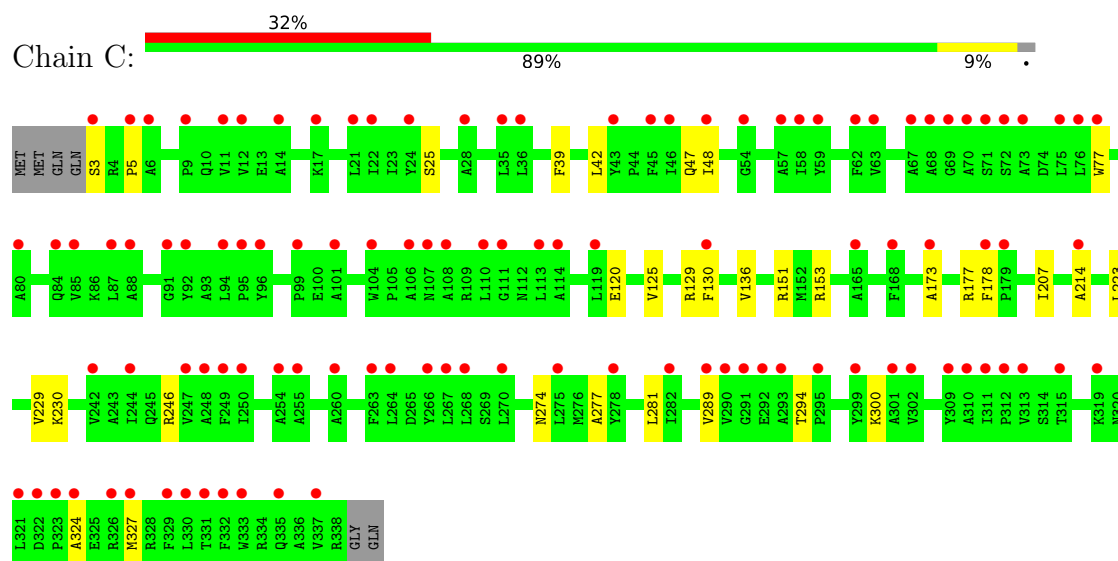
- Molecule 1: Iron ABC transporter, periplasmic iron-binding protein



- 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, α , β , γ	45.31Å 146.26Å 79.09Å 90.00° 99.89° 90.00°	Depositor
Resolution (Å)	73.24 – 2.15 73.24 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.3 (73.24-2.15) 95.3 (73.24-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.174 , 0.214 0.180 , 0.218	Depositor DCC
R_{free} test set	2565 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8484	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% 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: PDO, CIT, EDO, CO2, PGR

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	1.23	6/2726 (0.2%)	1.38	10/3696 (0.3%)
1	B	1.25	5/2723 (0.2%)	1.38	3/3693 (0.1%)
1	C	1.03	1/2704 (0.0%)	1.30	1/3668 (0.0%)
All	All	1.18	12/8153 (0.1%)	1.35	14/11057 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	PRO	C-O	-6.66	1.15	1.23
1	B	71	SER	C-O	6.07	1.31	1.23
1	B	161	PRO	C-O	-6.02	1.16	1.24
1	A	321	LEU	C-O	-5.92	1.16	1.24
1	A	252	LYS	C-O	-5.61	1.17	1.24
1	C	294	THR	N-CA	5.57	1.50	1.45
1	A	256	HIS	CE1-NE2	5.48	1.38	1.32
1	B	204	GLU	CD-OE1	5.36	1.35	1.25
1	A	294	THR	N-CA	5.23	1.50	1.45
1	A	114	ALA	C-O	5.17	1.30	1.23
1	A	46	ILE	C-O	-5.09	1.18	1.24
1	B	252	LYS	C-O	-5.06	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	THR	CA-C-O	-8.21	111.51	122.51
1	A	141	GLU	CB-CG-CD	7.11	124.68	112.60
1	A	210	GLU	CB-CG-CD	6.87	124.28	112.60
1	B	288	THR	CA-C-O	-6.59	113.68	122.51
1	A	288	THR	O-C-N	6.43	131.25	122.83
1	A	288	THR	CA-C-N	6.04	131.26	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	THR	C-N-CA	6.04	131.26	122.69
1	B	204	GLU	CB-CA-C	6.04	120.81	110.79
1	B	5	PRO	CB-CA-C	6.03	118.90	111.12
1	A	287	GLU	CB-CG-CD	5.50	121.94	112.60
1	A	210	GLU	CB-CA-C	5.32	119.62	110.79
1	A	331	THR	N-CA-C	-5.26	105.55	111.28
1	C	178	PHE	CB-CA-C	5.05	116.91	110.34
1	A	81	MET	CA-C-O	-5.01	115.24	120.55

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	2661	0	2677	17	0
1	B	2658	0	2675	16	0
1	C	2645	0	2651	17	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0
3	A	16	0	24	2	0
4	A	5	0	8	0	0
5	B	5	0	8	2	0
6	B	3	0	0	0	0
7	A	219	0	0	2	0
7	B	217	0	0	1	0
7	C	16	0	0	1	0
All	All	8484	0	8058	50	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 3.

All (50) 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:49:GLU:OE1	7:A:501:HOH:O	2.06	0.73
1:B:24:TYR:HB2	1:B:76[B]:LEU:HD22	1.76	0.67
1:B:287:GLU:H	5:B:402:PGR:H2	1.64	0.60
1:A:288:THR:HB	3:A:402:EDO:O1	2.00	0.60
1:A:205:LYS:HD3	1:A:210:GLU:HG2	1.83	0.60
1:C:130:PHE:O	1:C:151:ARG:NH2	2.34	0.60
1:C:136:VAL:O	7:C:501:HOH:O	2.17	0.56
1:C:274:ASN:HA	1:C:289:VAL:HG13	1.89	0.55
1:A:76:LEU:HD22	1:A:76:LEU:N	2.23	0.54
1:B:5:PRO:HD2	1:B:42:LEU:HD21	1.89	0.54
1:A:288:THR:H	3:A:402:EDO:H22	1.72	0.53
1:C:39:PHE:HD2	1:C:48:ILE:HD11	1.74	0.52
1:C:125:VAL:HG22	1:C:214:ALA:HB3	1.92	0.51
1:A:39:PHE:HD2	1:A:48:ILE:HD11	1.76	0.51
1:C:277:ALA:CB	1:C:289:VAL:HG12	2.41	0.51
1:C:324:ALA:O	1:C:327:MET:HE2	2.12	0.50
1:B:230:LYS:N	1:B:230:LYS:HD2	2.28	0.49
1:C:25:SER:HA	1:C:77:TRP:O	2.12	0.49
1:C:223:LEU:HB3	1:C:281:LEU:HD13	1.95	0.49
1:A:25:SER:HA	1:A:77:TRP:O	2.12	0.48
1:C:277:ALA:CB	1:C:289:VAL:CG1	2.92	0.48
1:B:21:LEU:HD23	1:B:48:ILE:HD13	1.94	0.47
1:C:277:ALA:HB2	1:C:289:VAL:CG1	2.44	0.47
1:C:120:GLU:OE2	1:C:246:ARG:NE	2.45	0.47
1:B:3:SER:O	1:B:271:ARG:HD2	2.13	0.47
1:A:120:GLU:OE2	1:A:246:ARG:NE	2.47	0.46
1:A:3:SER:O	1:A:271:ARG:HD2	2.16	0.46
1:B:25:SER:HA	1:B:77:TRP:O	2.14	0.46
1:A:230:LYS:H	1:A:230:LYS:CD	2.30	0.45
1:B:120:GLU:OE2	1:B:246:ARG:NE	2.48	0.45
1:B:230:LYS:HD2	1:B:230:LYS:H	1.82	0.45
1:B:24:TYR:HB2	1:B:76[B]:LEU:CD2	2.44	0.44
1:B:55:THR:HB	1:B:80:ALA:HB2	1.99	0.44
1:A:232:LEU:HD12	1:A:232:LEU:HA	1.85	0.44
1:A:182:GLN:NE2	7:A:504:HOH:O	2.39	0.44
1:B:338:ARG:HE	1:B:338:ARG:HA	1.82	0.43
1:C:129:ARG:HD3	1:C:130:PHE:CZ	2.54	0.43
1:B:338:ARG:HE	1:B:338:ARG:CA	2.32	0.42
1:A:39:PHE:CD2	1:A:48:ILE:HD11	2.54	0.42
1:B:29:GLN:HG2	7:B:525:HOH:O	2.20	0.42
1:A:207:ILE:HG12	1:A:229:VAL:HG11	2.01	0.42
1:C:5:PRO:HD2	1:C:42:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:PRO:HD2	1:A:42:LEU:HD21	2.02	0.41
1:B:286:ARG:HA	5:B:402:PGR:H2	2.02	0.41
1:A:55:THR:HB	1:A:80:ALA:HB2	2.01	0.41
1:B:328:ARG:HH11	1:B:328:ARG:HG3	1.85	0.41
1:C:173:ALA:O	1:C:177:ARG:HG2	2.19	0.41
1:C:277:ALA:HB2	1:C:289:VAL:HG11	2.03	0.40
1:C:207:ILE:HG12	1:C:229:VAL:HG11	2.03	0.40
1:A:125:VAL:HG22	1:A:214:ALA:HB3	2.04	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	336/342 (98%)	330 (98%)	6 (2%)	0	100	100
1	B	336/342 (98%)	332 (99%)	4 (1%)	0	100	100
1	C	334/342 (98%)	330 (99%)	4 (1%)	0	100	100
All	All	1006/1026 (98%)	992 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	270/273 (99%)	263 (97%)	7 (3%)	40	43
1	B	270/273 (99%)	262 (97%)	8 (3%)	36	38
1	C	268/273 (98%)	263 (98%)	5 (2%)	50	56
All	All	808/819 (99%)	788 (98%)	20 (2%)	42	45

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	20	ARG
1	A	76	LEU
1	A	141	GLU
1	A	204	GLU
1	A	230	LYS
1	A	307	LYS
1	B	3	SER
1	B	47	GLN
1	B	48	ILE
1	B	204	GLU
1	B	252	LYS
1	B	292	GLU
1	B	335	GLN
1	B	338	ARG
1	C	3	SER
1	C	47	GLN
1	C	153	ARG
1	C	230	LYS
1	C	300	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	258	ASN
1	A	296	GLN
1	A	335	GLN
1	B	148	GLN
1	C	148	GLN
1	C	258	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	CIT	A	401	-	12,12,12	1.32	2 (16%)	17,17,17	1.09	1 (5%)
4	PDO	A	406	-	4,4,4	0.21	0	3,3,3	0.22	0
3	EDO	A	403	-	3,3,3	0.16	0	2,2,2	0.14	0
3	EDO	A	405	-	3,3,3	0.23	0	2,2,2	0.16	0
2	CIT	B	401	-	12,12,12	1.44	2 (16%)	17,17,17	0.96	0
5	PGR	B	402	-	4,4,4	0.62	0	4,4,4	0.66	0
6	CO2	B	403	-	2,2,2	0.23	0	1,1,1	0.93	0
3	EDO	A	402	-	3,3,3	0.21	0	2,2,2	0.41	0
3	EDO	A	404	-	3,3,3	0.14	0	2,2,2	0.18	0
2	CIT	C	401	-	12,12,12	1.18	1 (8%)	17,17,17	1.21	2 (11%)

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	CIT	A	401	-	-	2/16/16/16	-
4	PDO	A	406	-	-	1/2/2/2	-
3	EDO	A	403	-	-	1/1/1/1	-
3	EDO	A	405	-	-	1/1/1/1	-
2	CIT	B	401	-	-	3/16/16/16	-
5	PGR	B	402	-	-	2/2/2/2	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	A	404	-	-	1/1/1/1	-
2	CIT	C	401	-	-	3/16/16/16	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	CIT	C3-C6	3.22	1.56	1.53
2	A	401	CIT	O5-C6	2.53	1.30	1.22
2	A	401	CIT	C3-C6	2.26	1.55	1.53
2	C	401	CIT	C3-C6	2.22	1.55	1.53
2	B	401	CIT	O4-C5	-2.16	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	CIT	O5-C6-C3	-2.62	117.02	122.09
2	A	401	CIT	O3-C5-C4	-2.49	115.90	122.95
2	C	401	CIT	O6-C6-C3	2.47	117.88	113.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	406	PDO	O1-C1-C2-C3
5	B	402	PGR	O1-C1-C2-O2
3	A	403	EDO	O1-C1-C2-O2
5	B	402	PGR	O1-C1-C2-C3
3	A	405	EDO	O1-C1-C2-O2
2	C	401	CIT	C2-C3-C6-O6
2	C	401	CIT	C4-C3-C6-O6
3	A	404	EDO	O1-C1-C2-O2
2	C	401	CIT	O7-C3-C6-O6
2	B	401	CIT	O1-C1-C2-C3
2	B	401	CIT	O2-C1-C2-C3

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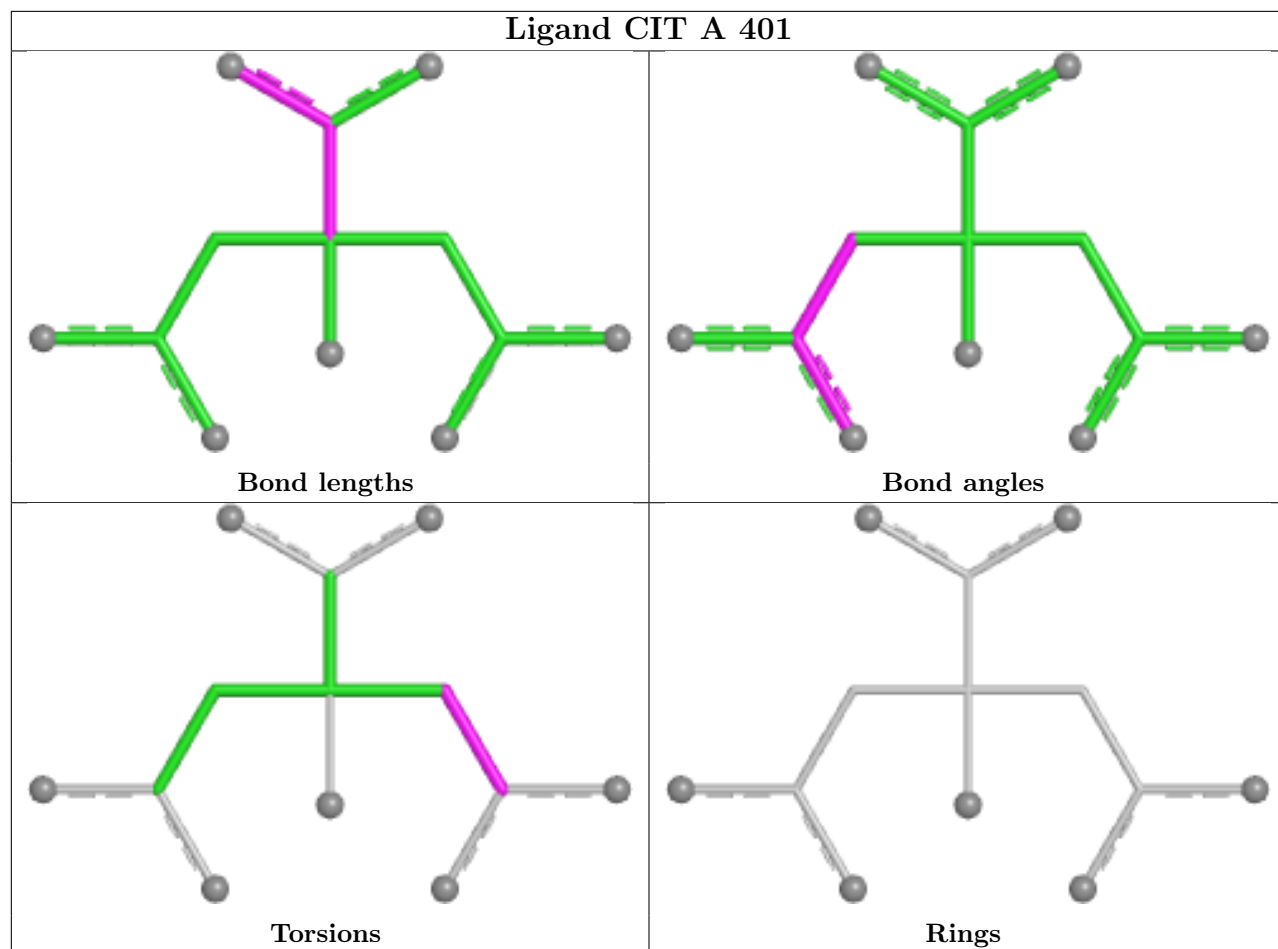
Mol	Chain	Res	Type	Atoms
2	B	401	CIT	C3-C4-C5-O3
2	A	401	CIT	O1-C1-C2-C3
2	A	401	CIT	O2-C1-C2-C3

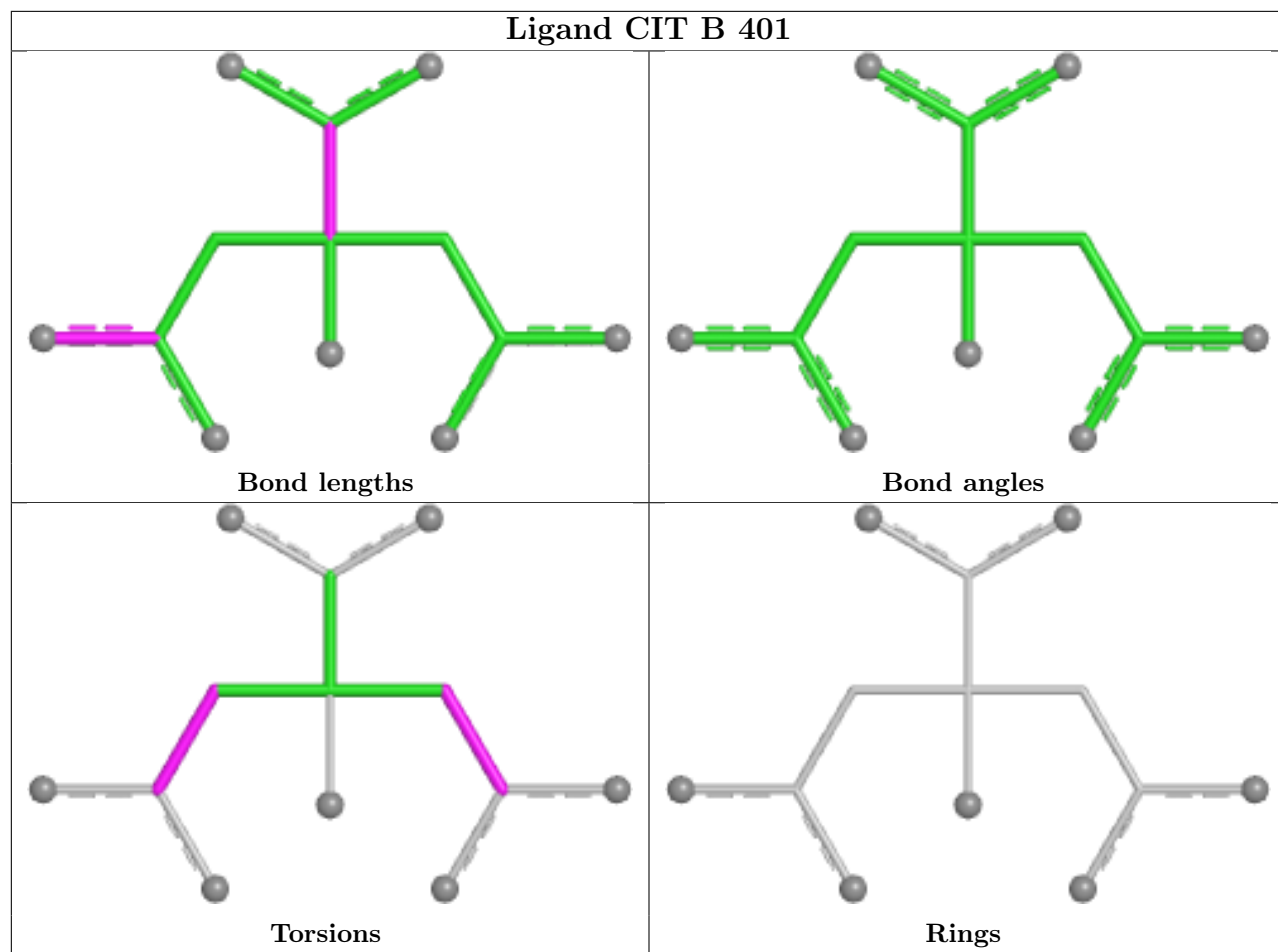
There are no ring outliers.

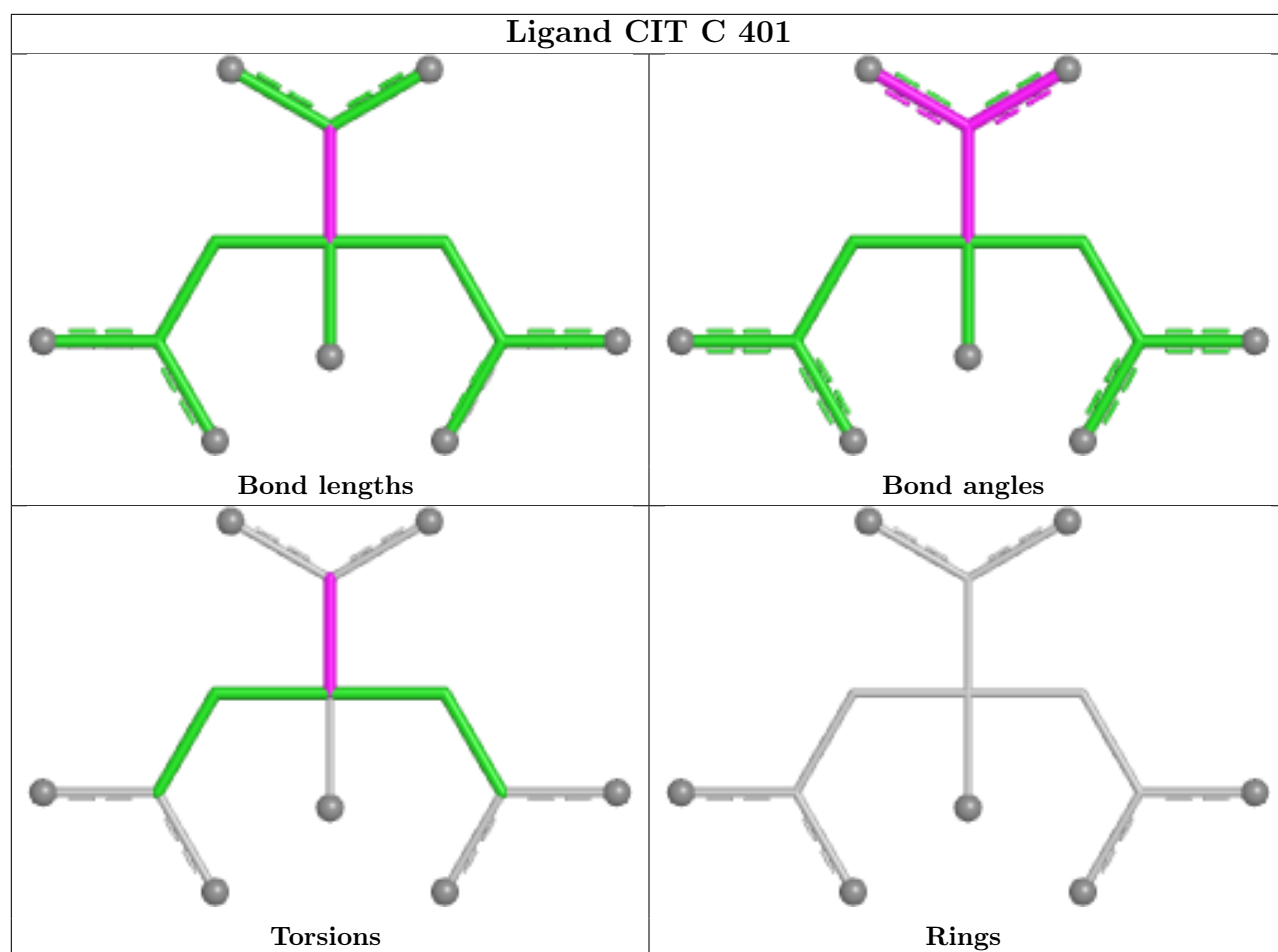
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	402	PGR	2	0
3	A	402	EDO	2	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, 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	336/342 (98%)	-0.47	2 (0%) 85 87	12, 25, 43, 74	2 (0%)
1	B	336/342 (98%)	-0.47	2 (0%) 85 87	11, 26, 46, 66	2 (0%)
1	C	336/342 (98%)	1.66	109 (32%) 1 1	46, 100, 161, 180	0
All	All	1008/1026 (98%)	0.24	113 (11%) 10 11	11, 33, 145, 180	4 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	321	LEU	4.5
1	C	324	ALA	4.5
1	C	290	VAL	4.4
1	C	67	ALA	4.1
1	C	94	LEU	3.8
1	C	45	PHE	3.8
1	A	71	SER	3.7
1	C	11	VAL	3.7
1	C	63	VAL	3.6
1	C	106	ALA	3.5
1	C	14	ALA	3.5
1	C	35	LEU	3.4
1	C	254	ALA	3.4
1	C	99	PRO	3.3
1	C	267	LEU	3.3
1	C	95	PRO	3.3
1	C	21	LEU	3.3
1	C	87	LEU	3.2
1	C	289	VAL	3.2
1	C	6	ALA	3.2
1	C	75	LEU	3.2
1	C	3	SER	3.2
1	C	70	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	165	ALA	3.1
1	C	46	ILE	3.1
1	C	76	LEU	3.1
1	C	59	TYR	3.0
1	C	278	TYR	3.0
1	C	331	THR	3.0
1	C	68	ALA	3.0
1	C	57	ALA	3.0
1	C	113	LEU	3.0
1	C	250	ILE	3.0
1	C	249	PHE	3.0
1	C	242	VAL	2.9
1	C	91	GLY	2.9
1	C	36	LEU	2.9
1	C	58	ILE	2.8
1	C	173	ALA	2.8
1	C	5	PRO	2.8
1	C	22	ILE	2.8
1	C	270	LEU	2.8
1	C	323	PRO	2.8
1	C	48	ILE	2.8
1	C	54	GLY	2.7
1	C	92	TYR	2.7
1	C	17	LYS	2.7
1	C	319	LYS	2.7
1	C	28	ALA	2.7
1	C	110	LEU	2.7
1	C	119	LEU	2.7
1	C	329	PHE	2.6
1	C	104	TRP	2.6
1	C	327	MET	2.6
1	B	3	SER	2.6
1	C	12	VAL	2.6
1	C	255	ALA	2.6
1	C	333	TRP	2.6
1	C	309	TYR	2.5
1	C	248	ALA	2.5
1	C	71	SER	2.5
1	C	275	LEU	2.5
1	C	62	PHE	2.5
1	C	311	ILE	2.5
1	C	96	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	179	PRO	2.4
1	C	130	PHE	2.4
1	C	263	PHE	2.4
1	C	291	GLY	2.4
1	C	247	VAL	2.4
1	C	315	THR	2.4
1	C	69	GLY	2.4
1	C	332	PHE	2.4
1	C	302	VAL	2.4
1	C	80	ALA	2.3
1	C	84	GLN	2.3
1	C	107	ASN	2.3
1	C	313	VAL	2.3
1	C	114	ALA	2.3
1	C	268	LEU	2.3
1	C	168	PHE	2.3
1	C	214	ALA	2.3
1	C	322	ASP	2.3
1	C	111	GLY	2.2
1	C	293	ALA	2.2
1	C	72	SER	2.2
1	C	73	ALA	2.2
1	C	24	TYR	2.2
1	C	9	PRO	2.1
1	C	310	ALA	2.1
1	C	337	VAL	2.1
1	C	326	ARG	2.1
1	C	101	ALA	2.1
1	C	108	ALA	2.1
1	C	264	LEU	2.1
1	C	295	PRO	2.1
1	C	312	PRO	2.1
1	C	77	TRP	2.1
1	C	178	PHE	2.1
1	C	88	ALA	2.1
1	C	301	ALA	2.1
1	C	266	TYR	2.1
1	C	282	ILE	2.1
1	C	85	VAL	2.1
1	C	260	ALA	2.1
1	C	292	GLU	2.0
1	C	330	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	335	GLN	2.0
1	C	244	ILE	2.0
1	A	3	SER	2.0
1	B	6	ALA	2.0
1	C	43	TYR	2.0
1	C	299	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

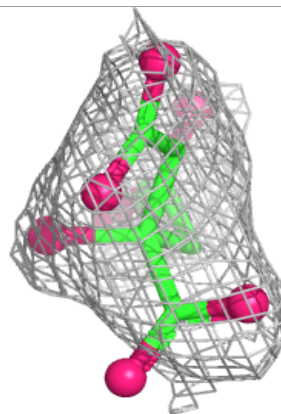
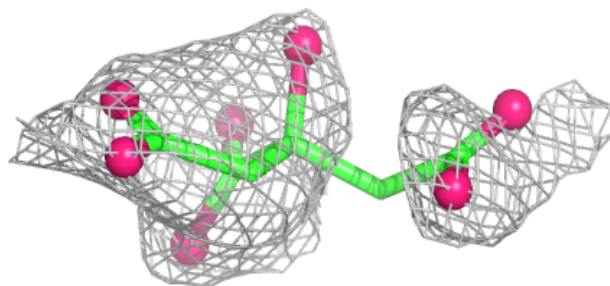
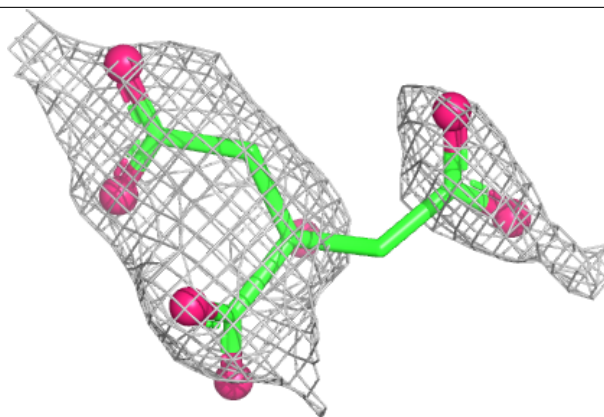
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	403	4/4	0.78	0.18	63,65,68,68	0
5	PGR	B	402	5/5	0.78	0.16	42,46,50,53	0
2	CIT	C	401	13/13	0.81	0.11	81,88,99,101	0
3	EDO	A	402	4/4	0.82	0.19	49,50,54,57	0
3	EDO	A	405	4/4	0.85	0.13	45,50,51,54	0
6	CO2	B	403	3/3	0.85	0.14	55,55,59,62	0
3	EDO	A	404	4/4	0.86	0.14	60,62,62,62	0
4	PDO	A	406	5/5	0.86	0.14	45,46,50,53	0
2	CIT	A	401	13/13	0.97	0.05	20,21,28,30	0
2	CIT	B	401	13/13	0.97	0.05	18,21,24,25	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.

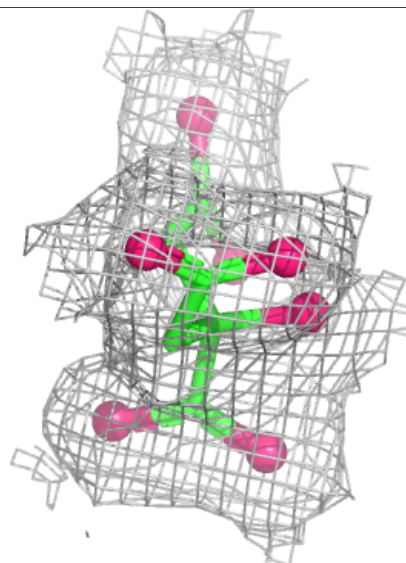
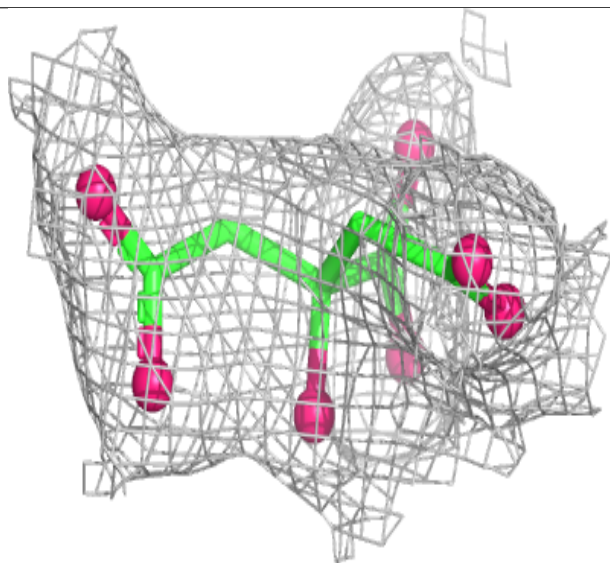
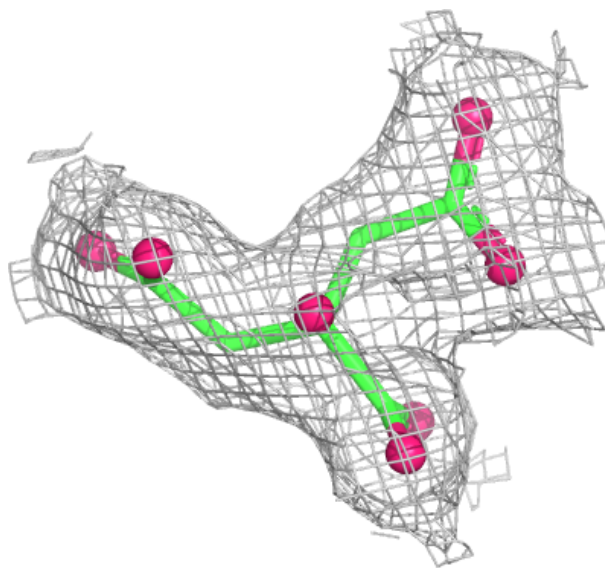
Electron density around CIT C 401:

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



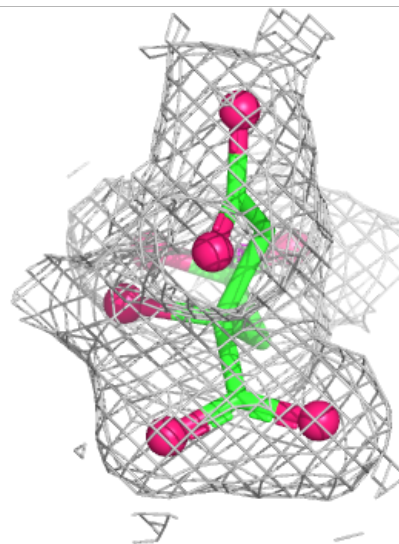
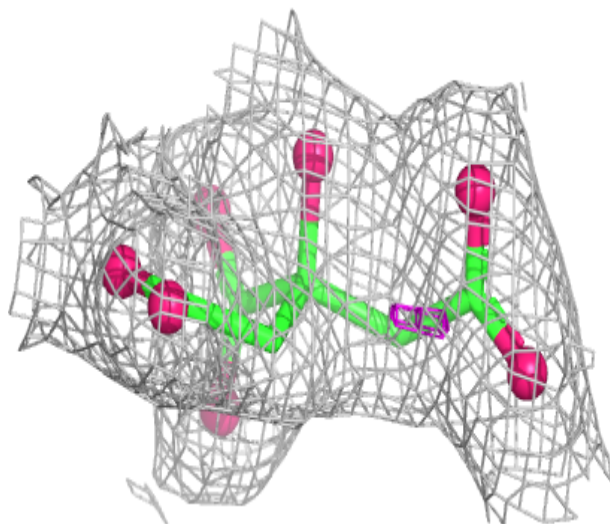
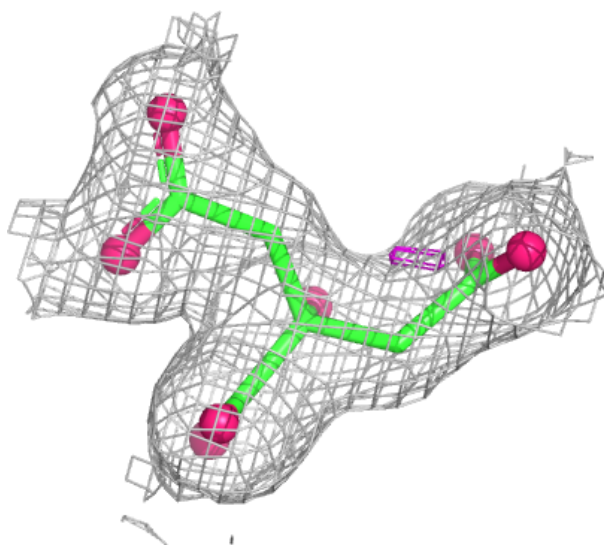
Electron density around CIT A 401:

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



Electron density around CIT 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.