



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 08:12 PM JST

PDB ID : 7F6P
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 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

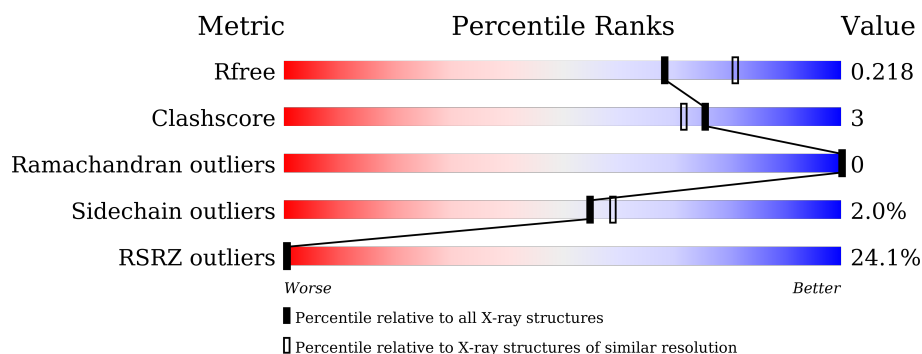
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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	<div> <div style="width: 89%;"></div> <div style="width: 8%;"></div> <div style="width: 5%;"></div> <div style="width: 2%;"></div> </div> <div>89% 8% ..</div>
1	B	342	<div> <div style="width: 89%;"></div> <div style="width: 8%;"></div> <div style="width: 5%;"></div> <div style="width: 2%;"></div> </div> <div>89% 8% ..</div>
1	C	342	<div> <div style="width: 71%;"></div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> </div> <div>71% 90% 8% .</div>

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.

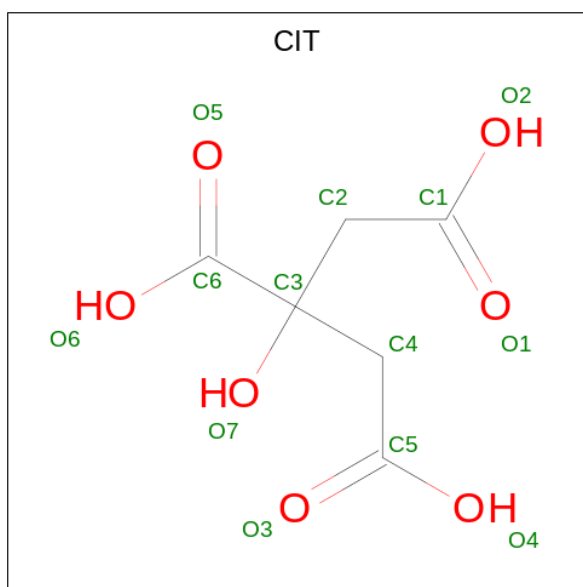
- Molecule 1 is a protein called Iron ABC transporter, periplasmic iron-binding protein.

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:

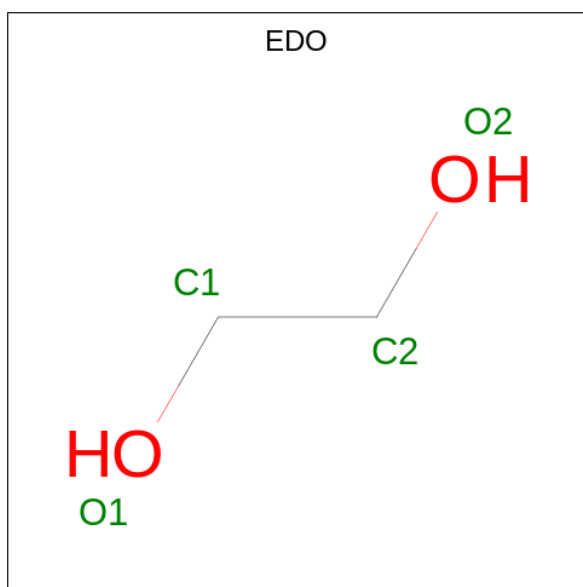
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q53VZ2
A	0	MET	-	expression tag	UNP Q53VZ2
A	28	ALA	ASP	engineered mutation	UNP Q53VZ2
B	-1	MET	-	initiating methionine	UNP Q53VZ2
B	0	MET	-	expression tag	UNP Q53VZ2
B	28	ALA	ASP	engineered mutation	UNP Q53VZ2
C	-1	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 (three-letter code: 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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



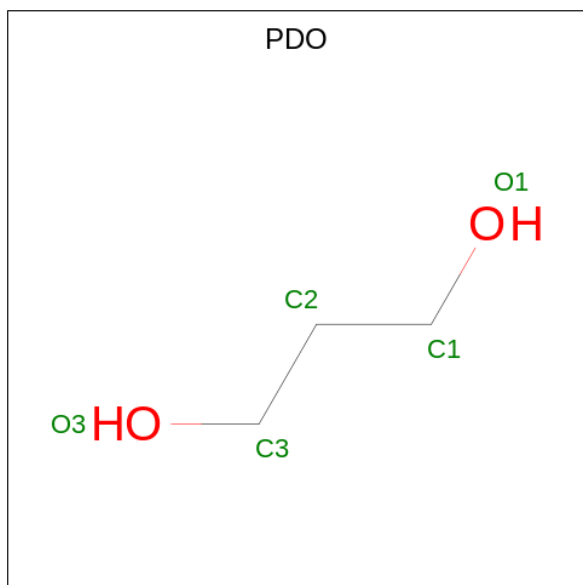
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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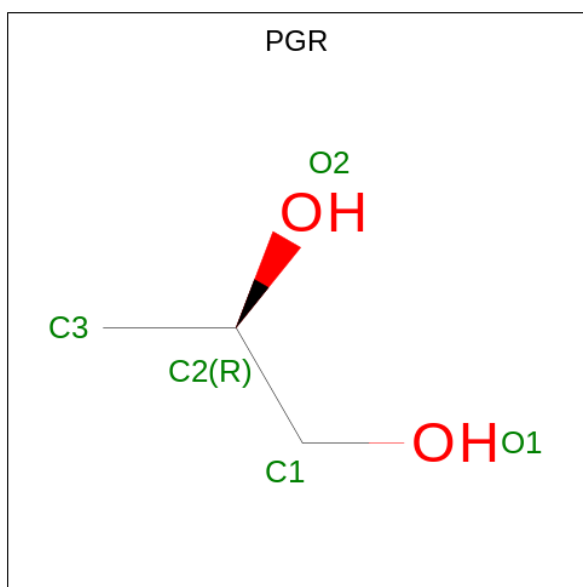
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,3-PROPANDIOL (three-letter code: PDO) (formula: $C_3H_8O_2$).



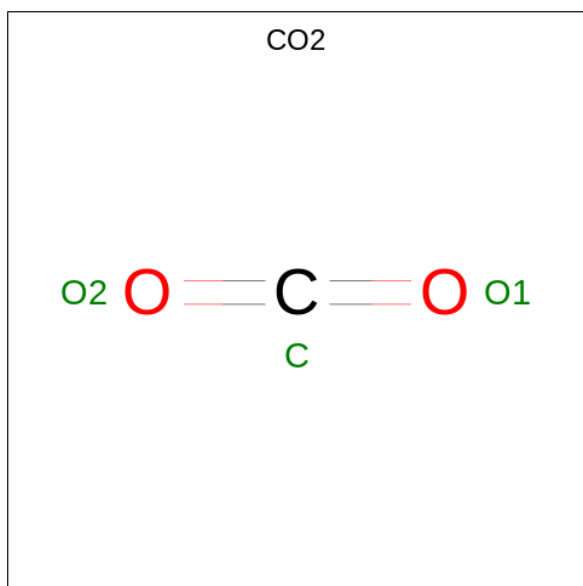
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 5 is R-1,2-PROPANEDIOL (three-letter code: 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 (three-letter code: CO2) (formula: CO₂).



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

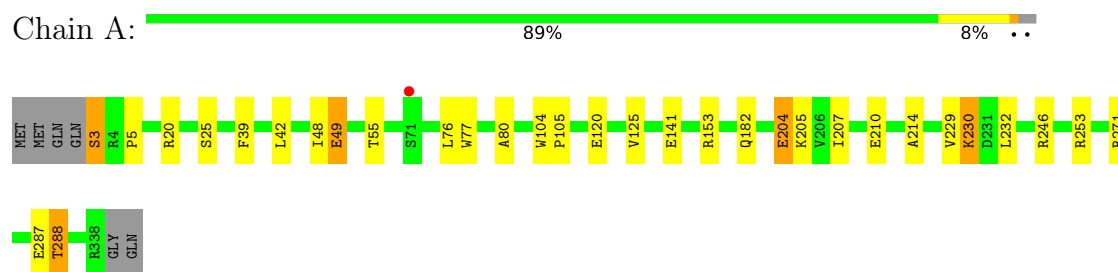
- Molecule 7 is water.

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

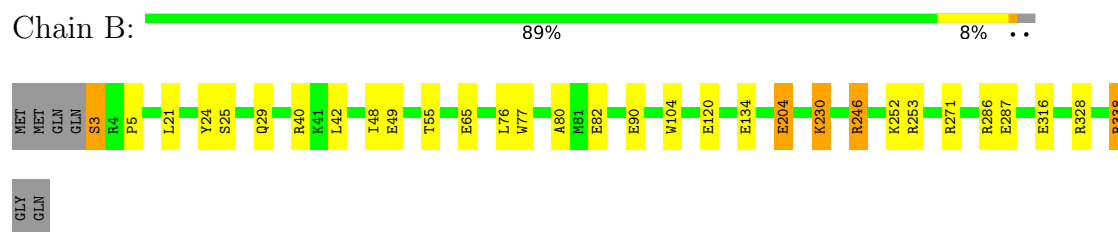
3 Residue-property plots [i](#)

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.

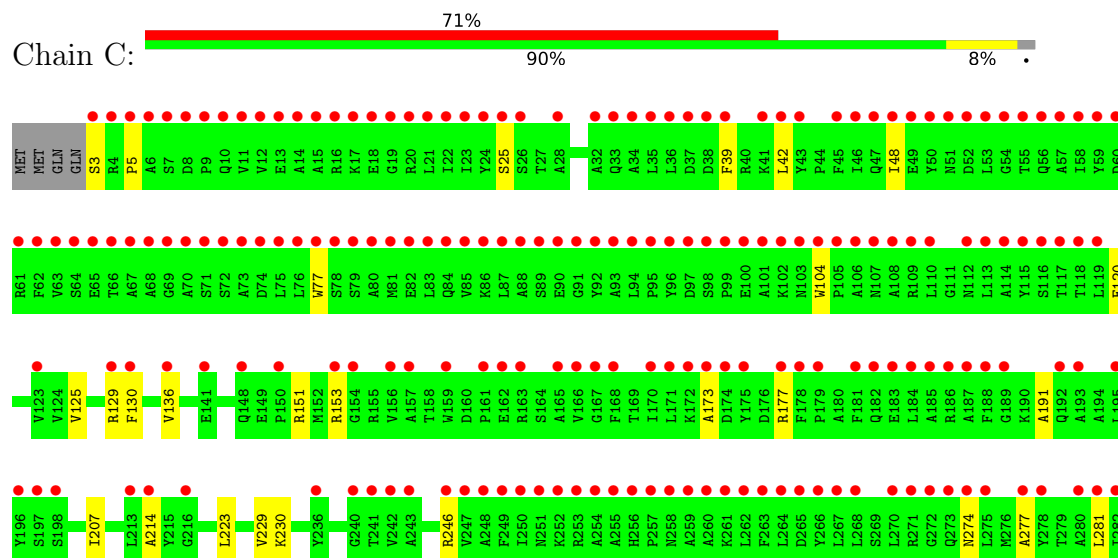
- Molecule 1: Iron ABC transporter, periplasmic iron-binding protein



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



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



F283	F284	F285	F286	F287	F288	F289	F290	F291	F292	F293	F296	F297	F298	F299	F300	F301	F302	F303	F306	F307	F308	F309	F310	F311	F312	F313	F314	F315	F316	F317	F318	F319	F320	F321	F322	F323	F324	F325	F326	F327	F328	F329	F330	F331	F332	F333	F334	F335	F336	F337	F338	GLY	GLN
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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 73.13 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.3 (73.24-2.15) 95.3 (73.13-2.15)	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 (4.89%)	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)	0.31 , 49.3	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGR, CO2, EDO, PDO, CIT

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	0.94	5/2726 (0.2%)	0.99	4/3696 (0.1%)
1	B	0.94	7/2723 (0.3%)	0.97	4/3693 (0.1%)
1	C	0.70	0/2704	0.83	1/3668 (0.0%)
All	All	0.87	12/8153 (0.1%)	0.93	9/11057 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	GLU	CD-OE1	8.98	1.35	1.25
1	B	49	GLU	CD-OE1	8.12	1.34	1.25
1	A	204	GLU	CD-OE1	7.54	1.33	1.25
1	A	287	GLU	CD-OE1	7.41	1.33	1.25
1	A	49	GLU	CD-OE2	7.22	1.33	1.25
1	A	49	GLU	CD-OE1	6.97	1.33	1.25
1	B	316	GLU	CD-OE2	-6.47	1.18	1.25
1	B	82	GLU	CD-OE2	6.08	1.32	1.25
1	A	141	GLU	CD-OE1	5.77	1.32	1.25
1	B	134	GLU	CD-OE2	5.16	1.31	1.25
1	B	65	GLU	CD-OE2	5.13	1.31	1.25
1	B	90	GLU	CD-OE2	5.01	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	253	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	253	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	191	ALA	CB-CA-C	5.89	118.93	110.10
1	B	40	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	288	THR	O-C-N	5.35	131.25	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	GLU	CB-CA-C	5.20	120.81	110.40
1	A	153	ARG	CG-CD-NE	-5.12	101.04	111.80
1	B	246	ARG	CG-CD-NE	-5.05	101.20	111.80

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	16	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	49	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 (49) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	264 (98%)	6 (2%)	52	55
1	B	270/273 (99%)	264 (98%)	6 (2%)	52	55
1	C	268/273 (98%)	264 (98%)	4 (2%)	65	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	808/819 (99%)	792 (98%)	16 (2%)	55 59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	20	ARG
1	A	104	TRP
1	A	105	PRO
1	A	204	GLU
1	A	230	LYS
1	B	3	SER
1	B	104	TRP
1	B	204	GLU
1	B	230	LYS
1	B	252	LYS
1	B	338	ARG
1	C	3	SER
1	C	104	TRP
1	C	153	ARG
1	C	230	LYS

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

Mol	Chain	Res	Type
1	B	47	GLN

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

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	$\# Z > 2$
6	CO2	B	403	-	2,2,2	0.24	0	1,1,1	0.87	0
5	PGR	B	402	-	3,4,4	0.24	0	1,4,4	0.04	0
3	EDO	A	405	-	3,3,3	0.23	0	2,2,2	0.23	0
2	CIT	C	401	-	3,12,12	0.56	0	3,17,17	0.91	0
4	PDO	A	406	-	4,4,4	0.21	0	3,3,3	0.21	0
3	EDO	A	403	-	3,3,3	0.17	0	2,2,2	0.22	0
3	EDO	A	404	-	3,3,3	0.14	0	2,2,2	0.24	0
2	CIT	B	401	-	3,12,12	0.51	0	3,17,17	0.99	0
3	EDO	A	402	-	3,3,3	0.21	0	2,2,2	0.50	0
2	CIT	A	401	-	3,12,12	0.74	0	3,17,17	0.70	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
5	PGR	B	402	-	-	2/2/2/2	-
3	EDO	A	405	-	-	1/1/1/1	-
2	CIT	C	401	-	-	0/6/16/16	-
4	PDO	A	406	-	-	1/2/2/2	-
3	EDO	A	403	-	-	1/1/1/1	-
3	EDO	A	404	-	-	1/1/1/1	-
2	CIT	B	401	-	-	0/6/16/16	-
3	EDO	A	402	-	-	0/1/1/1	-
2	CIT	A	401	-	-	0/6/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

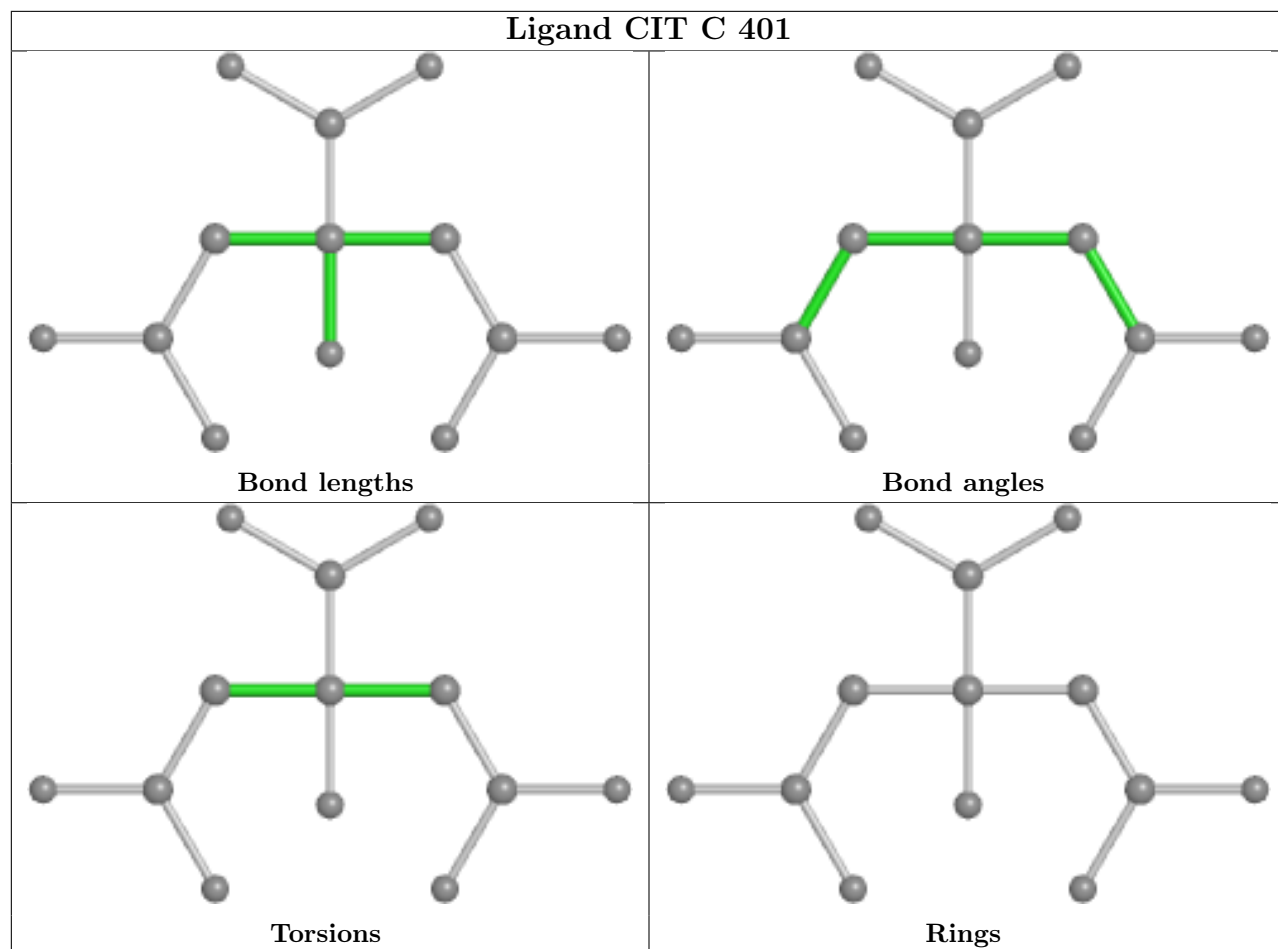
Mol	Chain	Res	Type	Atoms
4	A	406	PDO	O1-C1-C2-C3
5	B	402	PGR	O1-C1-C2-O2
3	A	403	EDO	O1-C1-C2-O2
5	B	402	PGR	O1-C1-C2-C3
3	A	405	EDO	O1-C1-C2-O2
3	A	404	EDO	O1-C1-C2-O2

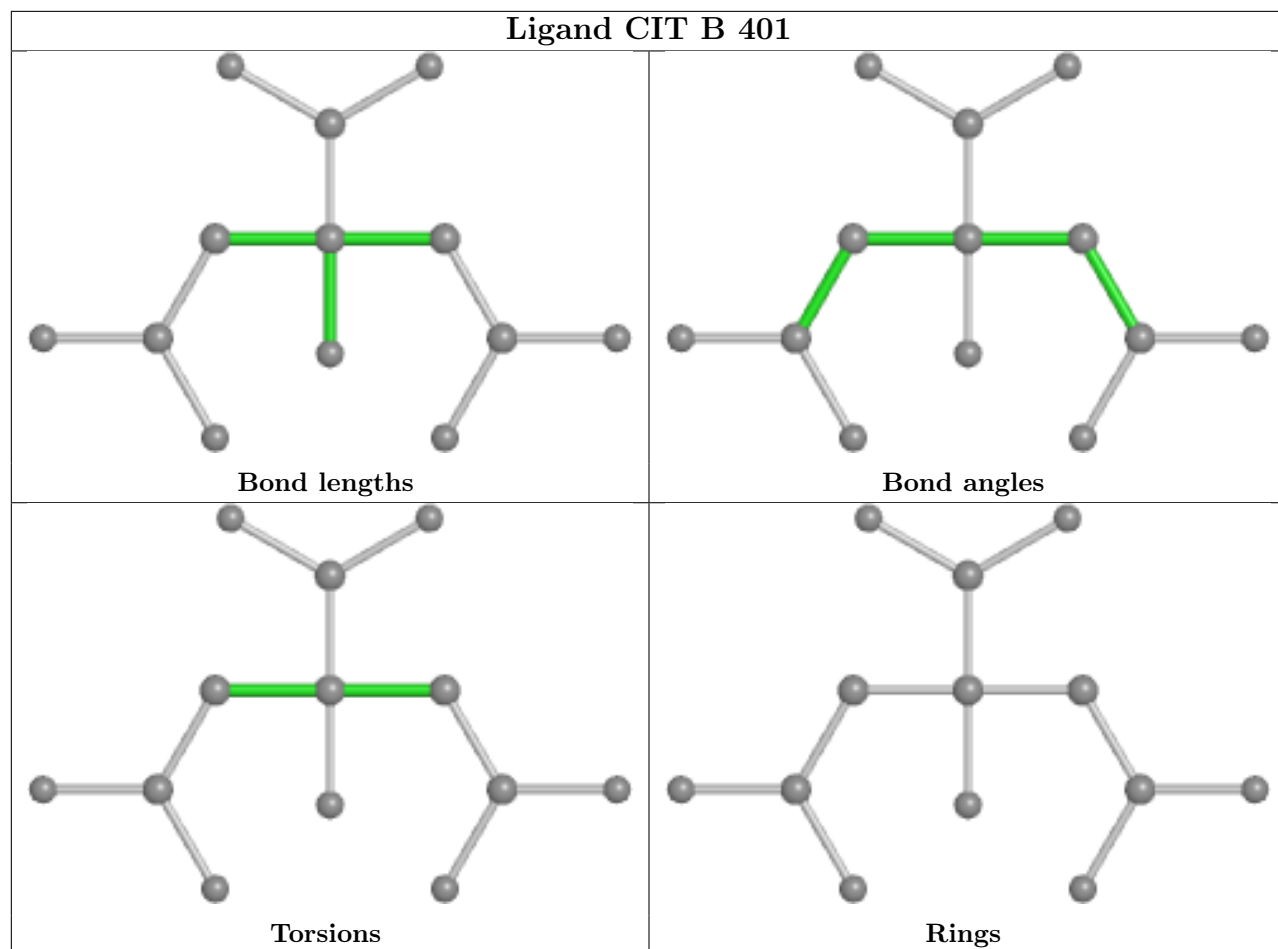
There are no ring outliers.

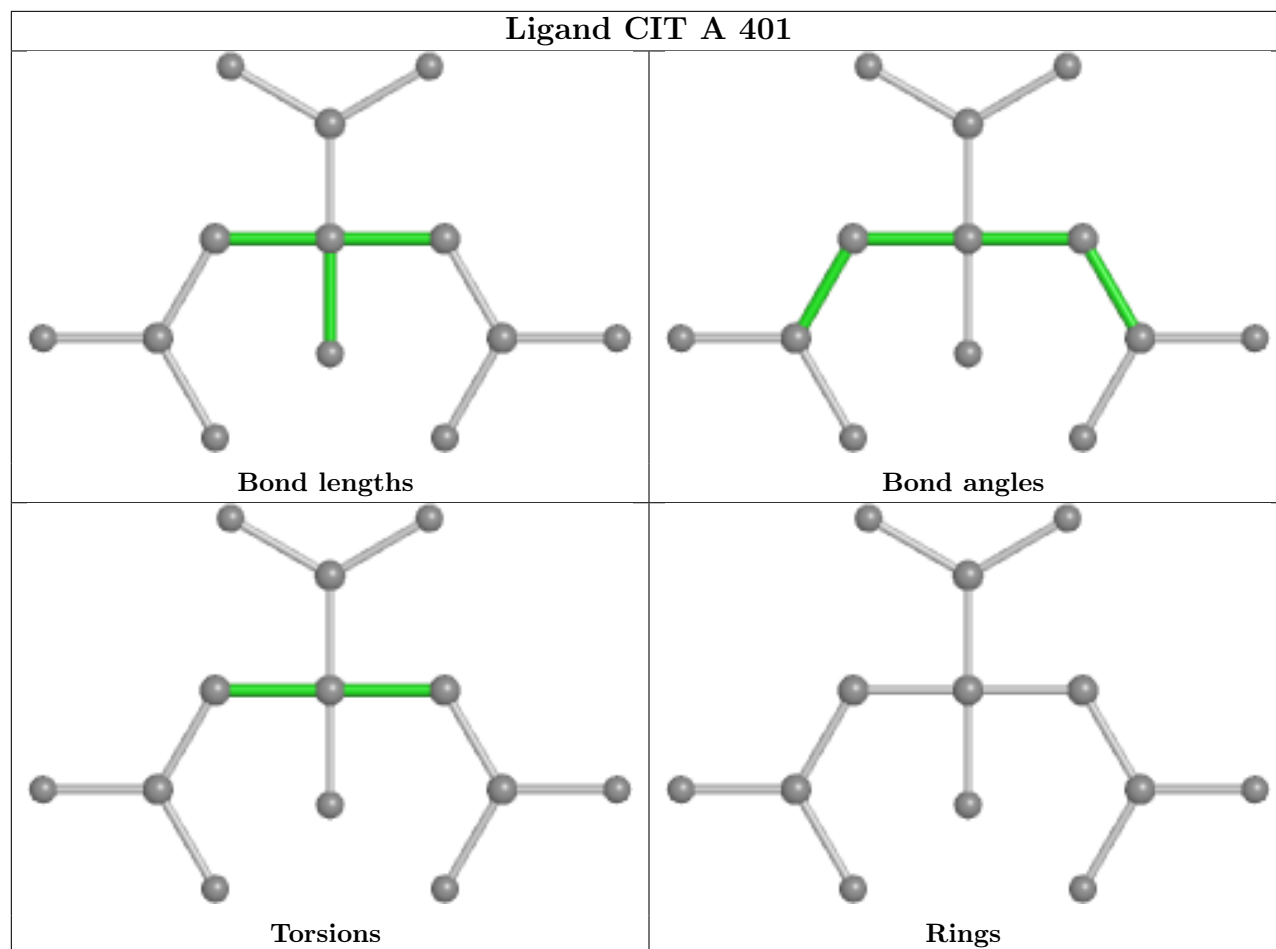
2 monomers are involved in 4 short contacts:

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%)	-0.05	1 (0%) 94 95	12, 25, 43, 74	0
1	B	336/342 (98%)	-0.07	0 100 100	13, 26, 46, 66	0
1	C	336/342 (98%)	3.78	242 (72%) 0 0	46, 100, 161, 180	0
All	All	1008/1026 (98%)	1.22	243 (24%) 0 0	12, 33, 145, 180	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	254	ALA	20.6
1	C	5	PRO	19.1
1	C	6	ALA	16.1
1	C	59	TYR	15.1
1	C	85	VAL	14.8
1	C	329	PHE	12.1
1	C	99	PRO	11.8
1	C	72	SER	11.3
1	C	4	ARG	11.1
1	C	333	TRP	11.0
1	C	324	ALA	10.9
1	C	96	TYR	10.6
1	C	253	ARG	10.4
1	C	3	SER	10.2
1	C	250	ILE	9.7
1	C	322	ASP	9.7
1	C	107	ASN	9.5
1	C	88	ALA	9.1
1	C	87	LEU	9.1
1	C	173	ALA	9.0
1	C	11	VAL	9.0
1	C	89	SER	8.9
1	C	46	ILE	8.9

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Mol	Chain	Res	Type	RSRZ
1	C	21	LEU	8.6
1	C	91	GLY	8.6
1	C	63	VAL	8.5
1	C	62	PHE	8.4
1	C	327	MET	8.2
1	C	108	ALA	7.9
1	C	93	ALA	7.9
1	C	75	LEU	7.8
1	C	92	TYR	7.7
1	C	321	LEU	7.5
1	C	94	LEU	7.3
1	C	35	LEU	6.9
1	C	95	PRO	6.9
1	C	67	ALA	6.8
1	C	7	SER	6.7
1	C	45	PHE	6.6
1	C	337	VAL	6.5
1	C	104	TRP	6.4
1	C	252	LYS	6.4
1	C	82	GLU	6.4
1	C	249	PHE	6.4
1	C	262	LEU	6.3
1	C	113	LEU	6.3
1	C	247	VAL	6.2
1	C	74	ASP	6.2
1	C	265	ASP	6.2
1	C	13	GLU	6.1
1	C	313	VAL	6.1
1	C	115	TYR	6.0
1	C	336	ALA	6.0
1	C	309	TYR	5.9
1	C	68	ALA	5.8
1	C	195	LEU	5.8
1	C	48	ILE	5.8
1	C	318	LEU	5.7
1	C	103	ASN	5.6
1	C	106	ALA	5.6
1	C	80	ALA	5.5
1	C	323	PRO	5.5
1	C	76	LEU	5.4
1	C	24	TYR	5.4
1	C	268	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	14	ALA	5.4
1	C	177	ARG	5.4
1	C	97	ASP	5.4
1	C	319	LYS	5.3
1	C	36	LEU	5.2
1	C	15	ALA	5.2
1	C	79	SER	5.2
1	C	338	ARG	5.1
1	C	73	ALA	5.1
1	C	286	ARG	5.1
1	C	50	TYR	5.1
1	C	317	ILE	5.0
1	C	263	PHE	5.0
1	C	12	VAL	5.0
1	C	287	GLU	5.0
1	C	288	THR	5.0
1	C	260	ALA	5.0
1	C	312	PRO	5.0
1	C	20	ARG	5.0
1	C	175	TYR	5.0
1	C	315	THR	5.0
1	C	331	THR	5.0
1	C	162	GLU	4.9
1	C	285	ARG	4.9
1	C	332	PHE	4.8
1	C	306	ASP	4.8
1	C	9	PRO	4.8
1	C	251	ASN	4.8
1	C	257	PRO	4.7
1	C	261	LYS	4.7
1	C	330	LEU	4.7
1	C	241	THR	4.7
1	C	178	PHE	4.7
1	C	248	ALA	4.7
1	C	58	ILE	4.6
1	C	255	ALA	4.6
1	C	163	ARG	4.6
1	C	174	ASP	4.6
1	C	311	ILE	4.6
1	C	335	GLN	4.6
1	C	83	LEU	4.6
1	C	114	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	170	ILE	4.5
1	C	118	THR	4.5
1	C	53	LEU	4.5
1	C	57	ALA	4.5
1	C	328	ARG	4.4
1	C	77	TRP	4.4
1	C	297	ALA	4.3
1	C	325	GLU	4.3
1	C	320	ASN	4.3
1	C	78	SER	4.3
1	C	8	ASP	4.3
1	C	168	PHE	4.3
1	C	105	PRO	4.2
1	C	256	HIS	4.2
1	C	47	GLN	4.2
1	C	66	THR	4.1
1	C	267	LEU	4.1
1	C	51	ASN	4.1
1	C	266	TYR	4.1
1	C	60	ASP	4.1
1	C	102	LYS	4.0
1	C	166	VAL	4.0
1	C	49	GLU	4.0
1	C	52	ASP	3.9
1	C	275	LEU	3.9
1	C	86	LYS	3.9
1	C	34	ALA	3.9
1	C	258	ASN	3.9
1	C	296	GLN	3.8
1	C	159	TRP	3.8
1	C	23	ILE	3.8
1	C	116	SER	3.8
1	C	290	VAL	3.8
1	C	69	GLY	3.8
1	C	187	ALA	3.8
1	C	157	ALA	3.7
1	C	98	SER	3.7
1	C	61	ARG	3.6
1	C	274	ASN	3.6
1	C	289	VAL	3.6
1	C	54	GLY	3.6
1	C	64	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	65	GLU	3.5
1	C	303	GLY	3.5
1	C	100	GLU	3.5
1	C	240	GLY	3.5
1	C	186	ARG	3.4
1	C	216	GLY	3.4
1	C	119	LEU	3.4
1	C	42	LEU	3.4
1	C	70	ALA	3.3
1	C	84	GLN	3.3
1	C	179	PRO	3.3
1	C	264	LEU	3.3
1	C	81	MET	3.3
1	C	182	GLN	3.3
1	C	273	GLN	3.3
1	C	172	LYS	3.3
1	C	242	VAL	3.3
1	C	148	GLN	3.2
1	C	90	GLU	3.2
1	C	183	GLU	3.2
1	C	308	VAL	3.2
1	C	192	GLN	3.1
1	C	271	ARG	3.1
1	C	301	ALA	3.1
1	C	184	LEU	3.1
1	C	19	GLY	3.1
1	C	302	VAL	3.1
1	C	197	SER	3.0
1	C	188	PHE	3.0
1	C	282	ILE	3.0
1	C	165	ALA	3.0
1	C	39	PHE	2.9
1	C	32	ALA	2.9
1	C	259	ALA	2.9
1	C	334	ARG	2.9
1	C	130	PHE	2.8
1	C	167	GLY	2.8
1	C	246	ARG	2.8
1	C	189	GLY	2.8
1	C	41	LYS	2.8
1	C	214	ALA	2.7
1	C	293	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	38	ASP	2.7
1	C	181	PHE	2.7
1	A	71	SER	2.7
1	C	18	GLU	2.7
1	C	307	LYS	2.7
1	C	278	TYR	2.6
1	C	277	ALA	2.6
1	C	292	GLU	2.6
1	C	284	ALA	2.6
1	C	291	GLY	2.6
1	C	161	PRO	2.6
1	C	28	ALA	2.6
1	C	56	GLN	2.6
1	C	326	ARG	2.5
1	C	71	SER	2.5
1	C	272	GLY	2.5
1	C	22	ILE	2.5
1	C	26	SER	2.5
1	C	101	ALA	2.5
1	C	281	LEU	2.5
1	C	16	ARG	2.4
1	C	150	PRO	2.4
1	C	243	ALA	2.4
1	C	129	ARG	2.4
1	C	37	ASP	2.4
1	C	17	LYS	2.4
1	C	110	LEU	2.3
1	C	55	THR	2.3
1	C	10	GLN	2.3
1	C	270	LEU	2.3
1	C	141	GLU	2.3
1	C	236	TYR	2.3
1	C	153	ARG	2.3
1	C	193	ALA	2.3
1	C	171	LEU	2.2
1	C	185	ALA	2.2
1	C	136	VAL	2.2
1	C	196	TYR	2.2
1	C	299	TYR	2.2
1	C	117	THR	2.2
1	C	156	VAL	2.1
1	C	33	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	198	SER	2.1
1	C	112	ASN	2.1
1	C	123	VAL	2.1
1	C	109	ARG	2.1
1	C	213	LEU	2.1
1	C	43	TYR	2.1
1	C	154	GLY	2.1
1	C	283	PHE	2.0
1	C	25	SER	2.0
1	C	280	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 [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.

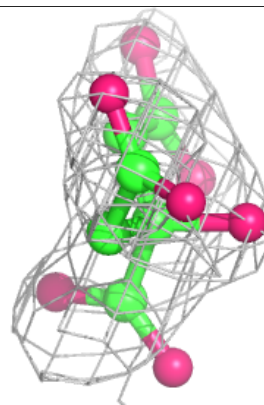
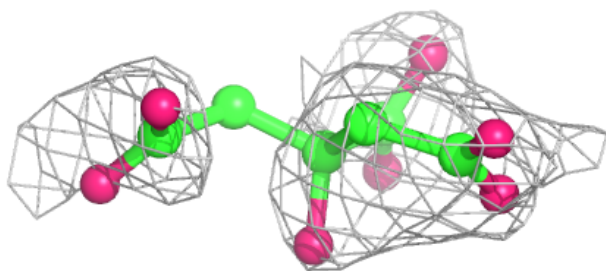
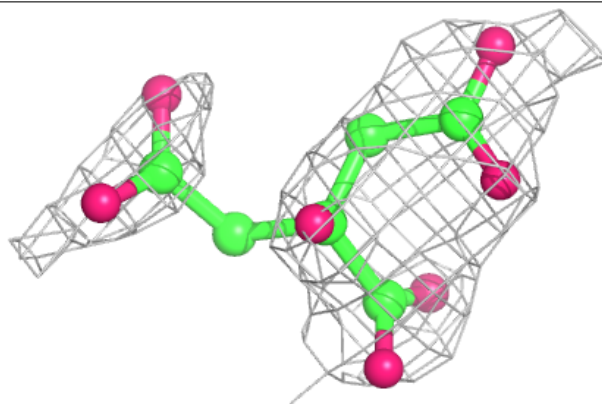
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PGR	B	402	5/5	0.63	0.24	42,46,50,53	0
3	EDO	A	404	4/4	0.71	0.19	60,62,62,62	0
3	EDO	A	405	4/4	0.75	0.18	45,50,51,54	0
3	EDO	A	402	4/4	0.75	0.26	49,50,54,57	0
2	CIT	C	401	13/13	0.81	0.23	81,88,99,101	0
6	CO2	B	403	3/3	0.86	0.13	55,55,59,62	0
3	EDO	A	403	4/4	0.89	0.16	63,65,68,68	0
4	PDO	A	406	5/5	0.92	0.18	45,46,50,53	0
2	CIT	A	401	13/13	0.96	0.11	20,21,28,30	0
2	CIT	B	401	13/13	0.97	0.11	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.

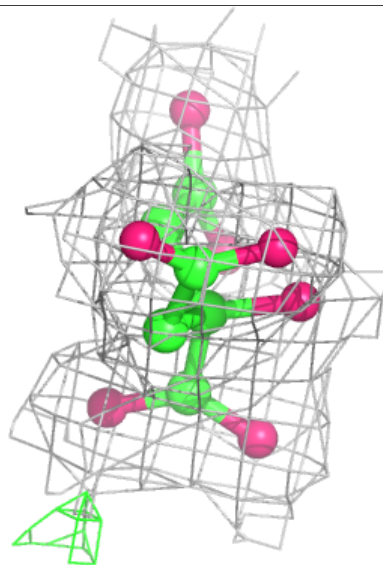
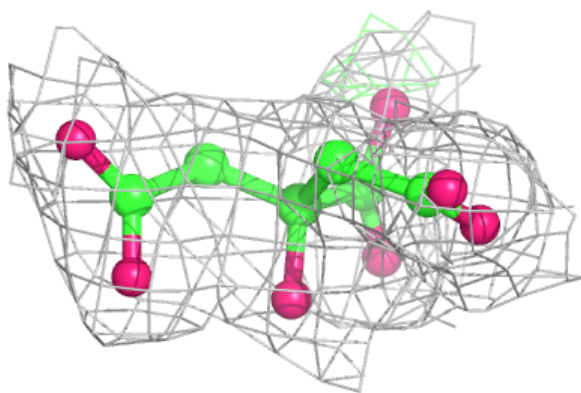
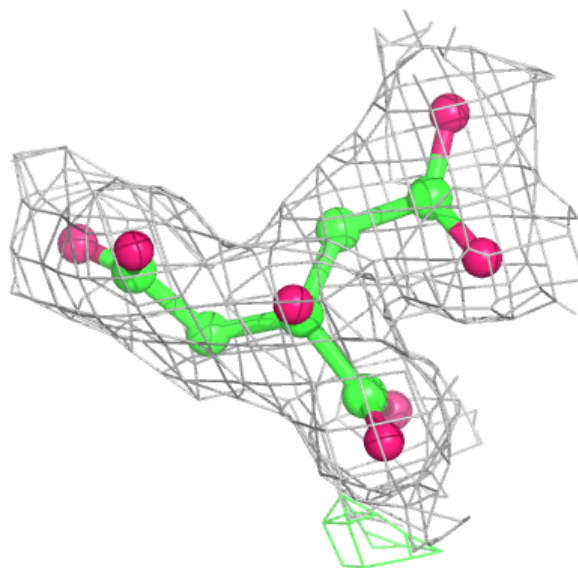
Electron density around CIT C 401:

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



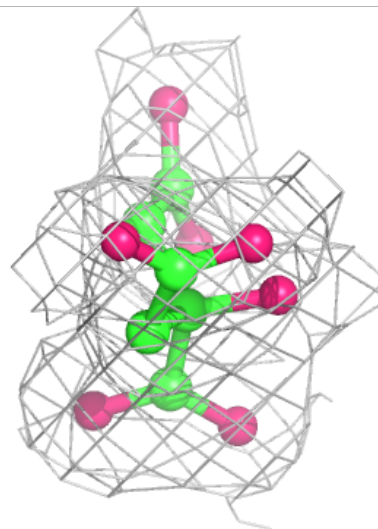
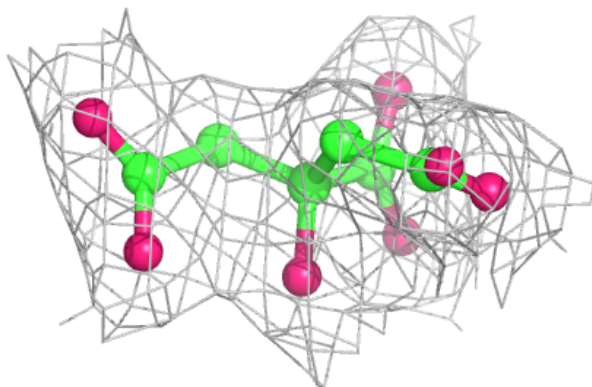
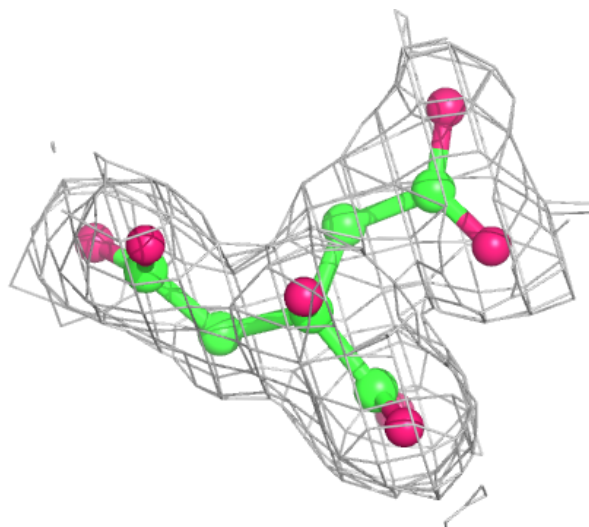
Electron density around CIT A 401:

$2mF_o-DF_c$ (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.