



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:31 AM UTC

PDB ID : 7F6K / pdb_00007f6k
Title : Crystal structure of metal-citrate-binding protein (MctA) of ABC transporter endogenously bound to citrate
Authors : Kanaujia, S.P.; Mandal, S.K.; Gogoi, P.
Deposited on : 2021-06-25
Resolution : 2.10 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

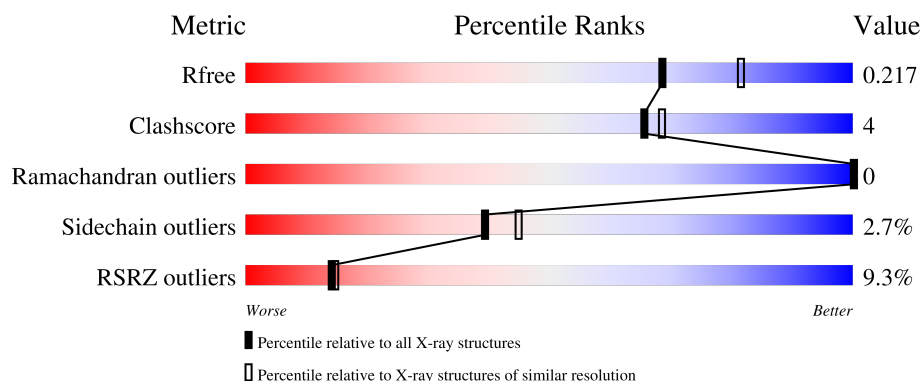
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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% 10% ..
1	B	342	88% 11% .
1	C	342	27% 87% 8% ...

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
4	MES	A	404	-	-	X	-
9	GOL	B	408	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8552 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	5	0
			2679	1716	468	491	4			
1	B	337	Total	C	N	O	S	0	7	0
			2689	1726	464	495	4			
1	C	330	Total	C	N	O	S	0	0	0
			2602	1669	449	480	4			

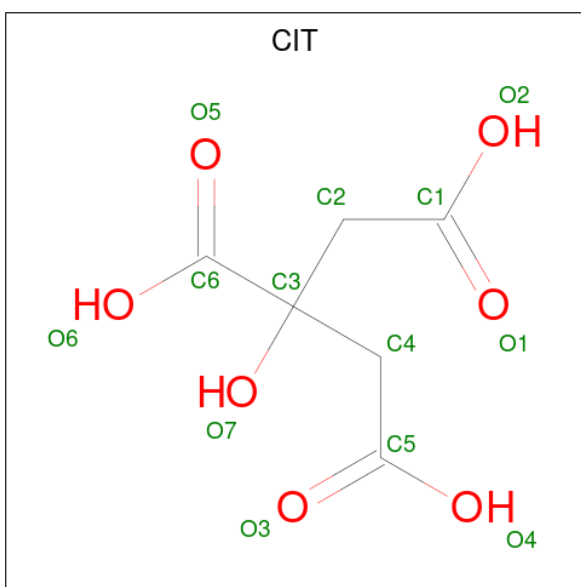
There are 6 discrepancies between the modelled and reference sequences:

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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

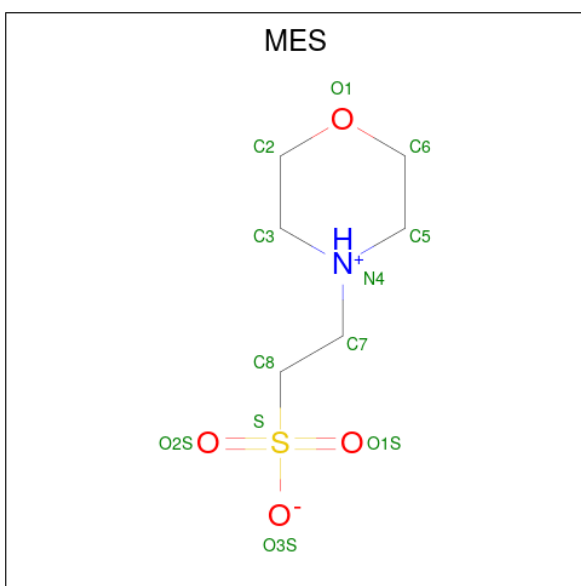
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cl	0	0
			2	2		
2	B	3	Total	Cl	0	0
			3	3		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇) (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 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



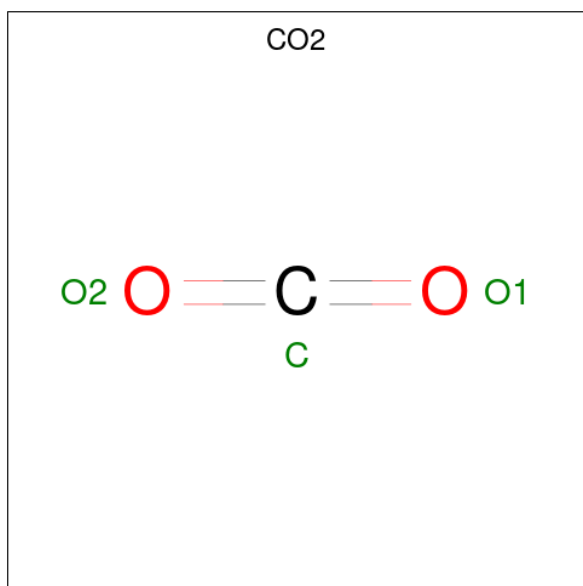
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is CARBON DIOXIDE (CCD ID: CO2) (formula: CO₂).



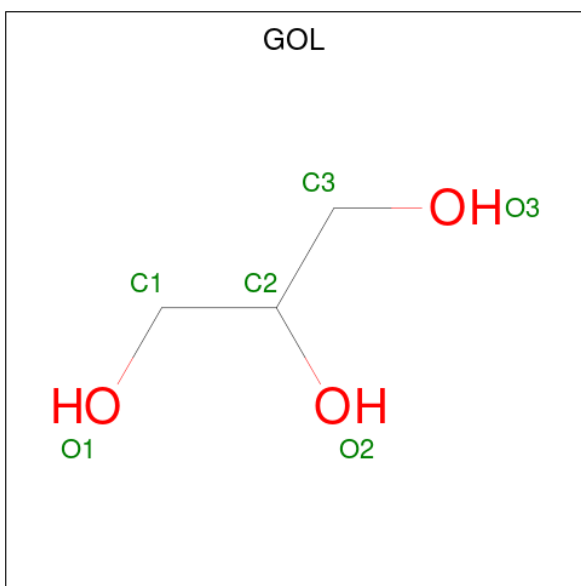
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			3	1	2		
7	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

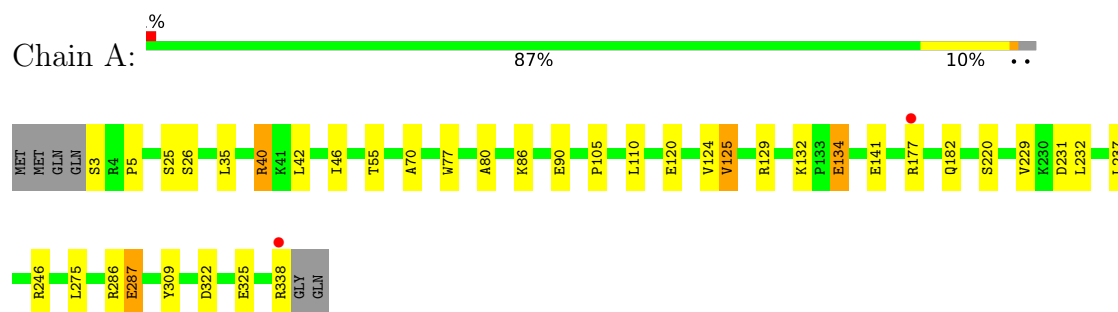
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	224	Total 224	O 224	0	0
10	B	228	Total 228	O 228	0	0
10	C	28	Total 28	O 28	0	0

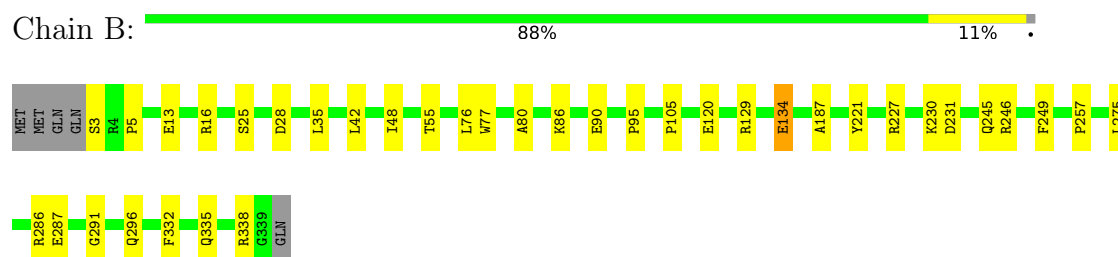
3 Residue-property plots

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

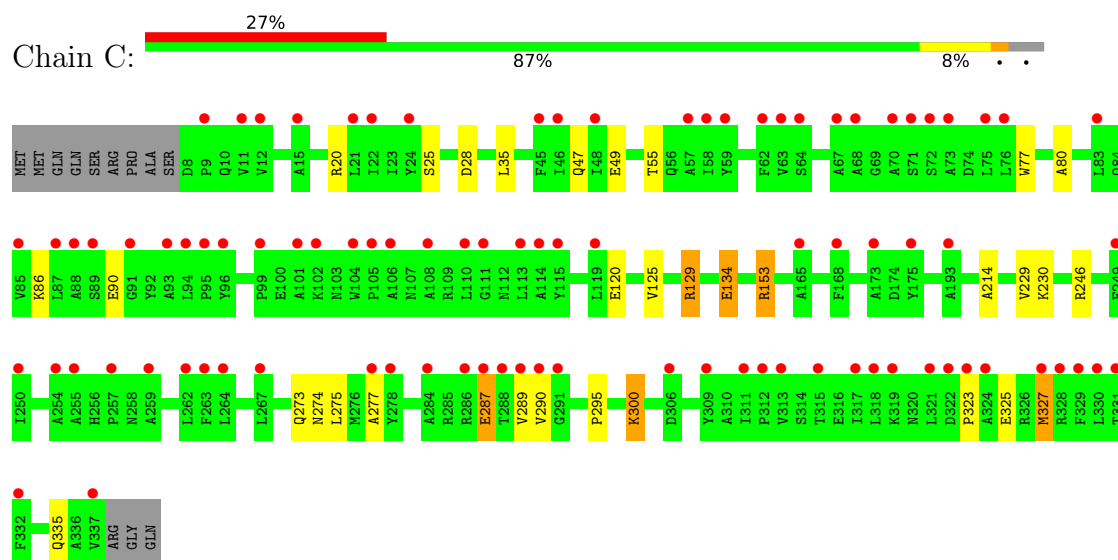
- Molecule 1: Iron ABC transporter, periplasmic iron-binding protein



- 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	45.55Å 145.11Å 79.24Å 90.00° 100.44° 90.00°	Depositor
Resolution (Å)	72.66 – 2.10 72.66 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (72.66-2.10) 100.0 (72.66-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.169 , 0.213 0.178 , 0.217	Depositor DCC
R_{free} test set	2893 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8552	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: ACT, MES, SO4, GOL, EDO, CO2, CIT, CL

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	1.22	5/2753 (0.2%)	1.32	5/3733 (0.1%)
1	B	1.20	3/2769 (0.1%)	1.32	3/3757 (0.1%)
1	C	1.05	0/2660	1.32	5/3609 (0.1%)
All	All	1.16	8/8182 (0.1%)	1.32	13/11099 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	SER	C-O	6.20	1.31	1.24
1	B	245	GLN	C-O	5.95	1.30	1.24
1	A	125[A]	VAL	C-O	5.77	1.29	1.24
1	A	125[B]	VAL	C-O	5.77	1.29	1.24
1	A	237	LEU	C-O	5.46	1.30	1.24
1	B	95	PRO	C-O	-5.37	1.17	1.23
1	B	257	PRO	C-O	-5.34	1.18	1.24
1	A	124	VAL	C-O	5.23	1.30	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	290	VAL	N-CA-C	11.66	125.26	106.72
1	C	290	VAL	CB-CA-C	-10.37	98.78	111.32
1	A	338	ARG	CA-C-O	-8.17	106.92	120.80
1	B	296	GLN	CB-CG-CD	7.16	124.77	112.60
1	A	325	GLU	CB-CA-C	6.91	123.35	110.70
1	A	325	GLU	N-CA-CB	-6.28	100.85	110.20
1	C	47	GLN	CB-CA-C	6.21	119.97	109.84
1	B	332	PHE	CA-CB-CG	-5.62	108.18	113.80
1	B	291	GLY	CA-C-O	-5.44	116.09	121.48
1	C	229	VAL	CA-C-N	5.08	127.34	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	229	VAL	C-N-CA	5.08	127.34	120.38
1	A	229	VAL	CA-C-N	5.06	127.56	120.28
1	A	229	VAL	C-N-CA	5.06	127.56	120.28

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	2679	0	2697	22	0
1	B	2689	0	2710	21	0
1	C	2602	0	2602	18	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
3	C	13	0	5	0	0
4	A	12	0	13	6	0
4	B	12	0	13	3	0
5	A	8	0	12	0	0
5	B	4	0	6	2	0
6	A	4	0	3	0	0
7	A	6	0	0	0	0
8	B	5	0	0	0	0
9	B	6	0	8	4	0
10	A	224	0	0	5	0
10	B	228	0	0	1	0
10	C	28	0	0	3	0
All	All	8552	0	8079	62	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 (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:GLU:H	4:B:406:MES:H81	1.23	1.04
1:A:141:GLU:HG3	10:A:630:HOH:O	1.69	0.93
1:A:322:ASP:HB2	10:A:696:HOH:O	1.69	0.93
1:A:287:GLU:H	4:A:404:MES:H81	1.52	0.74
1:A:129:ARG:NH1	1:A:231:ASP:OD2	2.24	0.71
1:B:76[B]:LEU:HD12	1:B:249:PHE:CZ	2.26	0.70
1:B:187:ALA:N	9:B:408:GOL:H31	2.07	0.70
1:A:125[B]:VAL:CG1	1:A:232:LEU:HD11	2.23	0.69
1:A:26:SER:O	10:A:502:HOH:O	2.15	0.63
1:B:105:PRO:HD3	4:B:406:MES:H52	1.81	0.61
1:C:287:GLU:HG3	1:C:295:PRO:HB2	1.82	0.60
1:B:129:ARG:NH1	1:B:231:ASP:OD2	2.33	0.60
1:A:287:GLU:H	4:A:404:MES:C8	2.16	0.58
1:B:25:SER:HA	1:B:77:TRP:O	2.03	0.58
1:A:35:LEU:HD23	1:A:275:LEU:HD22	1.86	0.58
1:C:35:LEU:HD23	1:C:275:LEU:HD22	1.87	0.57
1:C:25:SER:HA	1:C:77:TRP:O	2.06	0.56
1:B:187:ALA:HB2	9:B:408:GOL:H32	1.88	0.56
1:C:20:ARG:NH2	1:C:49:GLU:OE2	2.37	0.55
1:B:35:LEU:HD23	1:B:275[A]:LEU:HD22	1.89	0.54
1:C:323:PRO:O	1:C:327:MET:HE2	2.08	0.54
1:B:134:GLU:H	1:B:134:GLU:CD	2.16	0.54
1:A:25:SER:HA	1:A:77:TRP:O	2.08	0.54
1:A:134:GLU:H	1:A:134:GLU:CD	2.16	0.53
1:A:182:GLN:NE2	10:A:509:HOH:O	2.38	0.53
1:C:153:ARG:HB2	1:C:153:ARG:NH1	2.24	0.52
1:C:134:GLU:H	1:C:134:GLU:CD	2.16	0.52
1:B:28:ASP:OD1	10:B:501:HOH:O	2.19	0.52
1:A:5:PRO:HD2	1:A:42:LEU:HD21	1.92	0.51
1:B:5:PRO:HD2	1:B:42:LEU:HD21	1.94	0.48
1:C:274:ASN:HA	1:C:289:VAL:HG13	1.95	0.48
1:C:125:VAL:HG22	1:C:214:ALA:HB3	1.96	0.48
1:B:13:GLU:OE2	1:B:16:ARG:NH1	2.46	0.48
1:A:287:GLU:HB2	4:A:404:MES:H81	1.95	0.48
1:A:105:PRO:HD3	4:A:404:MES:H31	1.97	0.47
1:B:221:TYR:HB3	5:B:407:EDO:H22	1.95	0.47
1:A:70:ALA:O	10:A:503:HOH:O	2.20	0.46
1:C:273:GLN:HB3	1:C:289:VAL:HG21	1.98	0.45
4:A:404:MES:H52	4:A:404:MES:H82	1.57	0.45
1:B:187:ALA:HB2	9:B:408:GOL:C3	2.46	0.45
1:B:55:THR:HB	1:B:80:ALA:HB2	1.98	0.44
1:C:120:GLU:OE2	1:C:246:ARG:NE	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLU:OE2	1:B:246:ARG:NE	2.49	0.44
1:C:28:ASP:OD1	10:C:501:HOH:O	2.21	0.44
1:A:55:THR:HB	1:A:80:ALA:HB2	1.99	0.44
1:C:129:ARG:NH1	10:C:503:HOH:O	2.51	0.43
1:C:153:ARG:HB2	1:C:153:ARG:CZ	2.47	0.43
1:C:300:LYS:CE	10:C:520:HOH:O	2.66	0.43
1:C:86:LYS:O	1:C:90:GLU:HG3	2.18	0.43
1:A:286:ARG:HA	4:A:404:MES:H82	1.99	0.43
1:A:40:ARG:NH2	1:A:46:ILE:O	2.52	0.43
1:C:277:ALA:CB	1:C:289:VAL:CG1	2.98	0.42
1:A:120:GLU:OE2	1:A:246:ARG:NE	2.51	0.42
1:B:86:LYS:O	1:B:90:GLU:HG3	2.19	0.42
1:A:5:PRO:CD	1:A:42:LEU:HD21	2.51	0.41
1:A:86:LYS:O	1:A:90:GLU:HG3	2.20	0.41
1:B:187:ALA:CA	9:B:408:GOL:H31	2.51	0.41
1:B:28:ASP:OD2	5:B:407:EDO:O2	2.33	0.41
1:C:55:THR:HB	1:C:80:ALA:HB2	2.01	0.41
1:A:177[B]:ARG:HD2	1:A:309:TYR:CG	2.56	0.41
1:B:13:GLU:CD	1:B:16:ARG:HH12	2.29	0.40
1:B:286:ARG:HA	4:B:406:MES:H82	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	339/342 (99%)	335 (99%)	4 (1%)	0	100	100
1	B	342/342 (100%)	336 (98%)	6 (2%)	0	100	100
1	C	328/342 (96%)	324 (99%)	4 (1%)	0	100	100
All	All	1009/1026 (98%)	995 (99%)	14 (1%)	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	274/274 (100%)	268 (98%)	6 (2%)	45	53
1	B	276/274 (101%)	268 (97%)	8 (3%)	37	42
1	C	264/274 (96%)	255 (97%)	9 (3%)	32	35
All	All	814/822 (99%)	791 (97%)	23 (3%)	39	43

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	40	ARG
1	A	110	LEU
1	A	132	LYS
1	A	134	GLU
1	A	287	GLU
1	B	3	SER
1	B	48	ILE
1	B	134	GLU
1	B	227	ARG
1	B	230	LYS
1	B	335[A]	GLN
1	B	335[B]	GLN
1	B	338	ARG
1	C	129	ARG
1	C	134	GLU
1	C	153	ARG
1	C	230	LYS
1	C	287	GLU
1	C	300	LYS
1	C	325	GLU
1	C	327	MET
1	C	335	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	258	ASN
1	B	29	GLN
1	B	33	GLN
1	B	258	ASN
1	C	148	GLN
1	C	226	GLN
1	C	258	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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$
3	CIT	C	402	-	12,12,12	1.17	1 (8%)	17,17,17	1.30	2 (11%)
7	CO2	A	408	-	2,2,2	0.28	0	1,1,1	1.39	0
8	SO4	B	405	-	4,4,4	0.32	0	6,6,6	0.09	0
4	MES	A	404	-	12,12,12	0.86	0	15,16,16	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CIT	B	404	-	12,12,12	1.34	1 (8%)	17,17,17	0.86	0
5	EDO	B	407	-	3,3,3	0.28	0	2,2,2	0.23	0
5	EDO	A	405	-	3,3,3	0.12	0	2,2,2	0.20	0
5	EDO	A	406	-	3,3,3	0.05	0	2,2,2	0.28	0
9	GOL	B	408	-	5,5,5	0.36	0	5,5,5	0.82	0
4	MES	B	406	-	12,12,12	0.88	0	15,16,16	1.07	2 (13%)
6	ACT	A	407	-	3,3,3	1.05	0	3,3,3	0.75	0
7	CO2	A	409	-	2,2,2	0.06	0	1,1,1	1.05	0
3	CIT	A	403	-	12,12,12	1.29	1 (8%)	17,17,17	0.99	1 (5%)

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
3	CIT	C	402	-	-	8/16/16/16	-
4	MES	A	404	-	-	3/6/14/14	0/1/1/1
3	CIT	B	404	-	-	6/16/16/16	-
5	EDO	B	407	-	-	1/1/1/1	-
5	EDO	A	405	-	-	0/1/1/1	-
5	EDO	A	406	-	-	0/1/1/1	-
9	GOL	B	408	-	-	2/4/4/4	-
4	MES	B	406	-	-	3/6/14/14	0/1/1/1
3	CIT	A	403	-	-	2/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	CIT	O6-C6	-2.55	1.21	1.30
3	A	403	CIT	O4-C5	-2.52	1.22	1.30
3	C	402	CIT	C3-C6	2.18	1.55	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	CIT	O5-C6-C3	-3.05	116.19	122.09
3	C	402	CIT	O6-C6-C3	2.49	117.91	113.14
4	B	406	MES	C2-C3-N4	2.16	113.40	110.12
3	A	403	CIT	O5-C6-C3	-2.03	118.17	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	406	MES	C6-C5-N4	2.02	113.19	110.12

There are no chirality outliers.

All (25) torsion outliers are listed below:

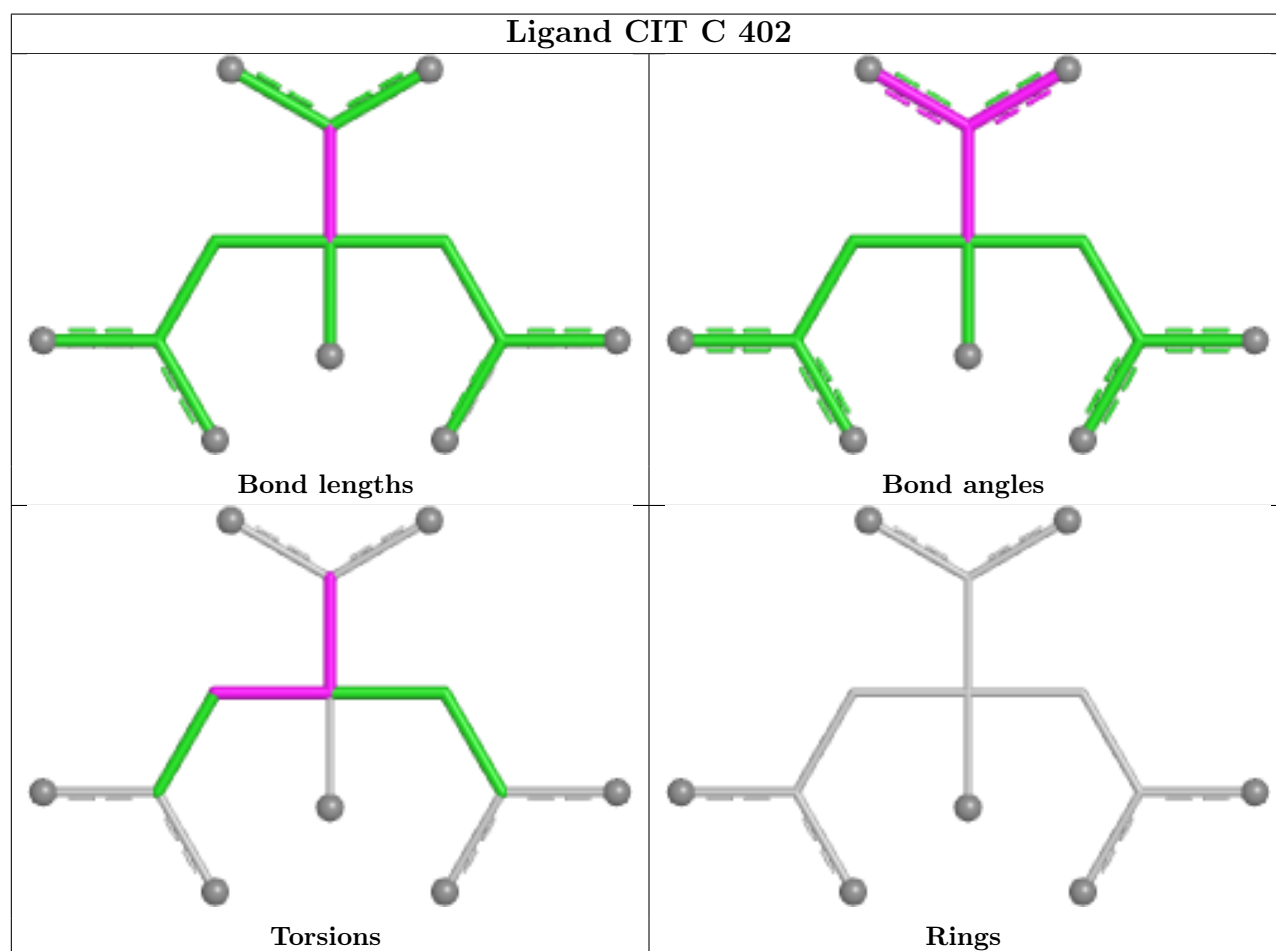
Mol	Chain	Res	Type	Atoms
4	A	404	MES	C8-C7-N4-C5
4	A	404	MES	N4-C7-C8-S
4	B	406	MES	C8-C7-N4-C3
4	B	406	MES	C8-C7-N4-C5
4	B	406	MES	N4-C7-C8-S
9	B	408	GOL	C1-C2-C3-O3
9	B	408	GOL	O2-C2-C3-O3
5	B	407	EDO	O1-C1-C2-O2
4	A	404	MES	C8-C7-N4-C3
3	C	402	CIT	C2-C3-C6-O6
3	C	402	CIT	C2-C3-C6-O5
3	C	402	CIT	C4-C3-C6-O5
3	C	402	CIT	C4-C3-C6-O6
3	B	404	CIT	C4-C3-C6-O5
3	B	404	CIT	C4-C3-C6-O6
3	C	402	CIT	O7-C3-C6-O5
3	C	402	CIT	O7-C3-C6-O6
3	B	404	CIT	O1-C1-C2-C3
3	C	402	CIT	C6-C3-C4-C5
3	A	403	CIT	C3-C4-C5-O3
3	B	404	CIT	C3-C4-C5-O3
3	B	404	CIT	O2-C1-C2-C3
3	C	402	CIT	C2-C3-C4-C5
3	B	404	CIT	C3-C4-C5-O4
3	A	403	CIT	C3-C4-C5-O4

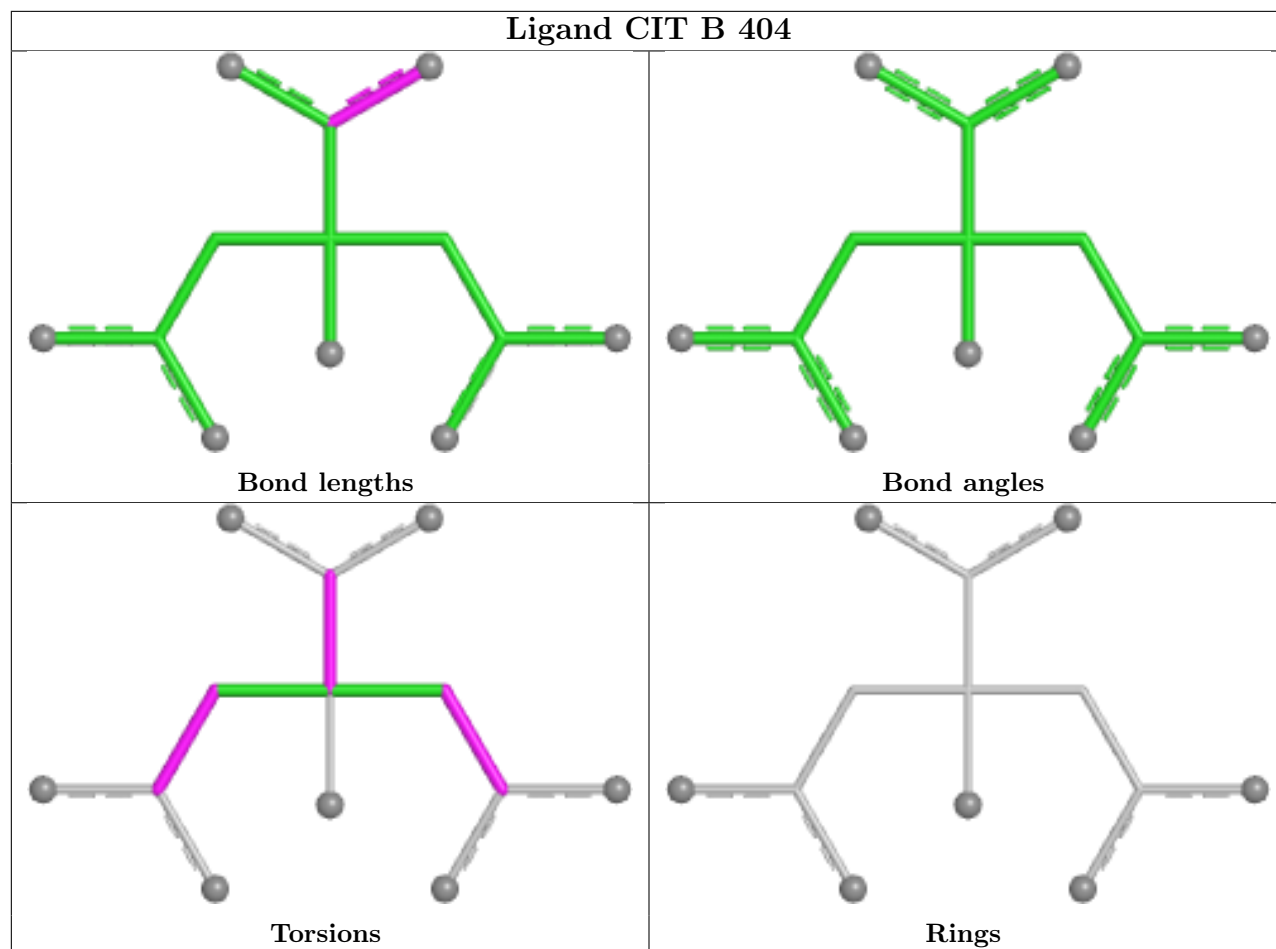
There are no ring outliers.

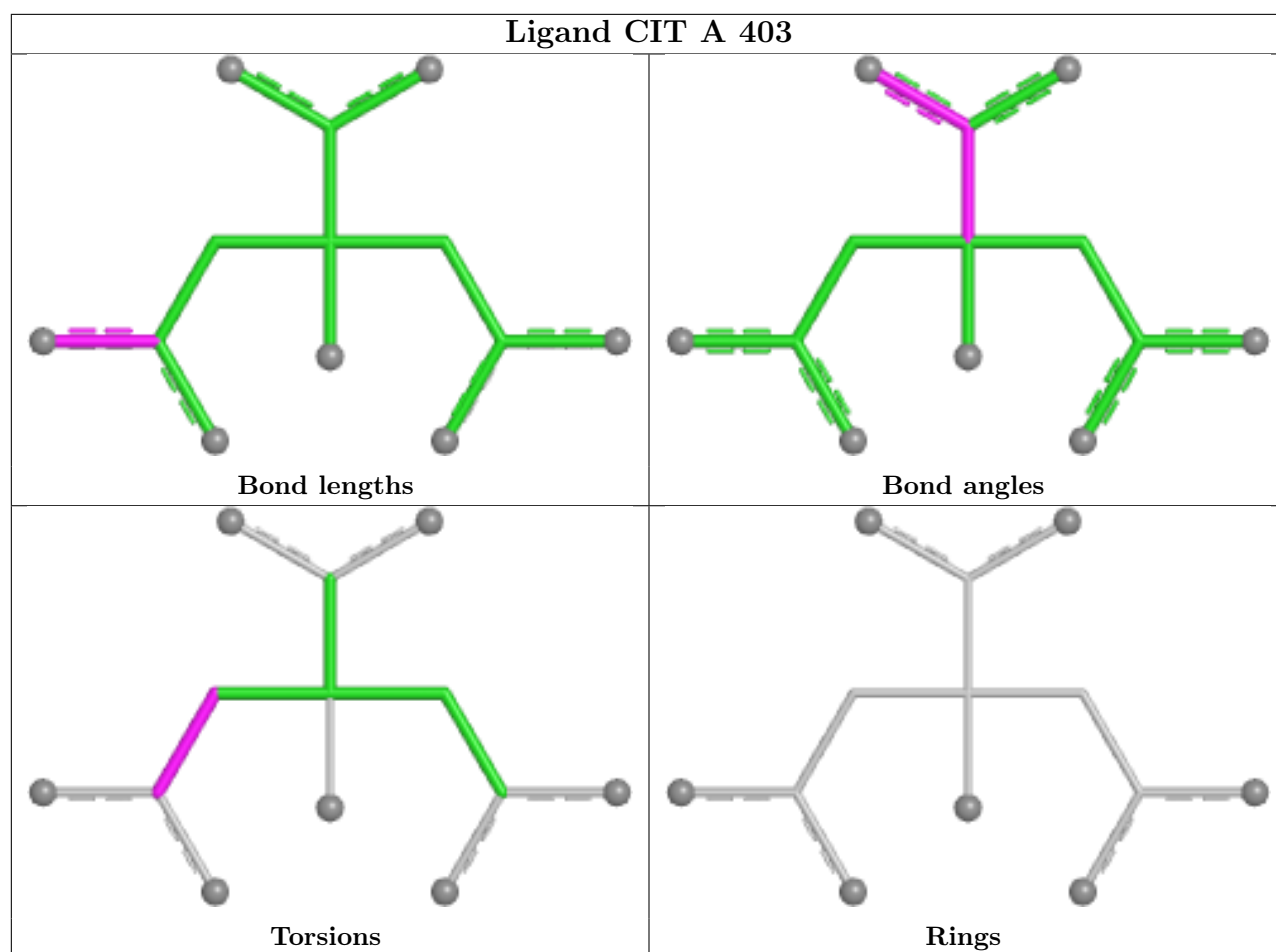
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	MES	6	0
5	B	407	EDO	2	0
9	B	408	GOL	4	0
4	B	406	MES	3	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%)	-0.49	2 (0%) 85 87	13, 22, 39, 66	5 (1%)
1	B	337/342 (98%)	-0.53	0 100 100	10, 22, 39, 64	7 (2%)
1	C	330/342 (96%)	1.49	91 (27%) 1 1	34, 73, 121, 136	0
All	All	1003/1026 (97%)	0.15	93 (9%) 14 15	10, 27, 108, 136	12 (1%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	290	VAL	6.0
1	C	324	ALA	4.8
1	C	67	ALA	4.0
1	C	288	THR	4.0
1	C	113	LEU	3.9
1	C	11	VAL	3.7
1	C	94	LEU	3.7
1	C	106	ALA	3.6
1	C	70	ALA	3.5
1	C	254	ALA	3.5
1	C	330	LEU	3.5
1	C	105	PRO	3.4
1	C	291	GLY	3.4
1	C	59	TYR	3.4
1	C	278	TYR	3.4
1	C	68	ALA	3.4
1	C	321	LEU	3.4
1	C	323	PRO	3.3
1	C	255	ALA	3.3
1	C	58	ILE	3.2
1	C	99	PRO	3.2
1	C	48	ILE	3.1
1	C	110	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	318	LEU	2.9
1	C	12	VAL	2.9
1	C	165	ALA	2.9
1	C	262	LEU	2.8
1	C	311	ILE	2.8
1	C	312	PRO	2.8
1	C	286	ARG	2.8
1	C	91	GLY	2.8
1	C	22	ILE	2.8
1	C	63	VAL	2.8
1	C	317	ILE	2.8
1	C	72	SER	2.8
1	C	327	MET	2.8
1	C	45	PHE	2.7
1	C	264	LEU	2.7
1	C	309	TYR	2.7
1	C	71	SER	2.7
1	C	88	ALA	2.7
1	C	315	THR	2.7
1	C	168	PHE	2.6
1	C	332	PHE	2.6
1	C	93	ALA	2.6
1	C	250	ILE	2.5
1	C	337	VAL	2.5
1	C	96	TYR	2.5
1	C	87	LEU	2.5
1	C	287	GLU	2.4
1	C	263	PHE	2.4
1	C	46	ILE	2.4
1	C	289	VAL	2.4
1	C	306	ASP	2.4
1	C	115	TYR	2.4
1	C	111	GLY	2.4
1	C	64	SER	2.4
1	C	57	ALA	2.4
1	C	173	ALA	2.4
1	C	284	ALA	2.4
1	C	24	TYR	2.3
1	C	76	LEU	2.3
1	C	267	LEU	2.3
1	C	102	LYS	2.3
1	C	329	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	313	VAL	2.3
1	C	114	ALA	2.3
1	C	249	PHE	2.3
1	C	85	VAL	2.3
1	C	104	TRP	2.3
1	C	95	PRO	2.3
1	C	62	PHE	2.2
1	C	193	ALA	2.2
1	C	277	ALA	2.2
1	C	89	SER	2.2
1	A	338	ARG	2.2
1	C	259	ALA	2.1
1	C	75	LEU	2.1
1	C	175	TYR	2.1
1	A	177[A]	ARG	2.1
1	C	73	ALA	2.1
1	C	319	LYS	2.1
1	C	15	ALA	2.1
1	C	108	ALA	2.1
1	C	9	PRO	2.1
1	C	257	PRO	2.1
1	C	331	THR	2.1
1	C	83	LEU	2.0
1	C	322	ASP	2.0
1	C	328	ARG	2.0
1	C	101	ALA	2.0
1	C	21	LEU	2.0
1	C	119	LEU	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,

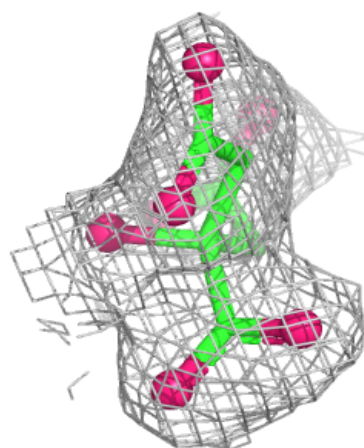
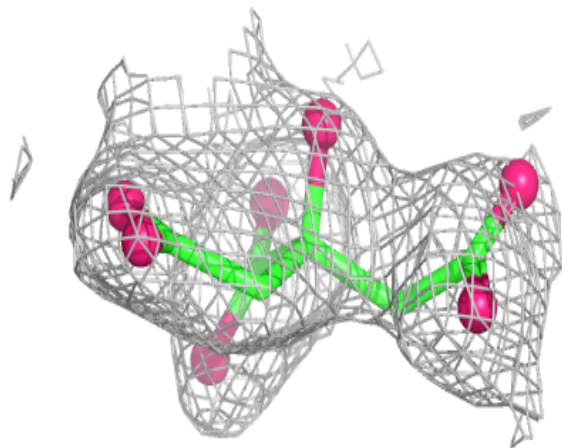
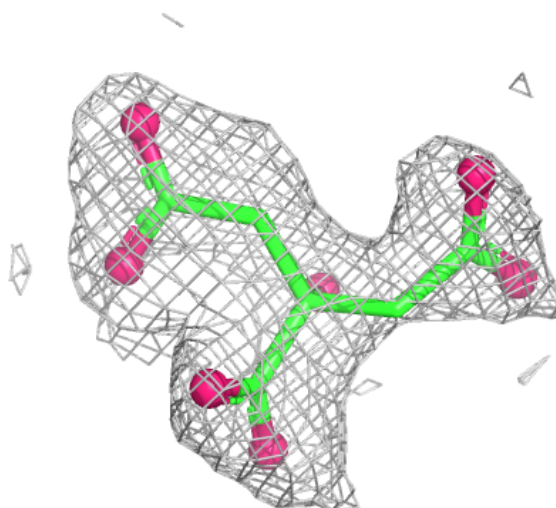
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ACT	A	407	4/4	0.75	0.20	56,60,61,62	0
3	CIT	C	402	13/13	0.81	0.11	53,57,68,74	0
5	EDO	B	407	4/4	0.83	0.12	37,43,45,46	0
5	EDO	A	405	4/4	0.85	0.12	46,47,49,52	0
7	CO2	A	408	3/3	0.85	0.13	34,34,39,48	0
9	GOL	B	408	6/6	0.85	0.16	30,37,41,43	0
2	CL	B	403	1/1	0.87	0.16	69,69,69,69	0
7	CO2	A	409	3/3	0.89	0.15	42,42,44,47	0
5	EDO	A	406	4/4	0.89	0.14	49,51,51,52	0
2	CL	A	402	1/1	0.91	0.11	56,56,56,56	0
4	MES	A	404	12/12	0.92	0.13	36,47,51,56	0
2	CL	C	401	1/1	0.93	0.08	63,63,63,63	0
2	CL	A	401	1/1	0.94	0.09	56,56,56,56	0
4	MES	B	406	12/12	0.95	0.10	39,45,49,51	0
2	CL	B	402	1/1	0.96	0.10	54,54,54,54	0
2	CL	B	401	1/1	0.97	0.07	46,46,46,46	0
8	SO4	B	405	5/5	0.97	0.09	44,45,46,46	0
3	CIT	B	404	13/13	0.97	0.05	15,17,18,19	0
3	CIT	A	403	13/13	0.98	0.04	17,19,21,22	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.

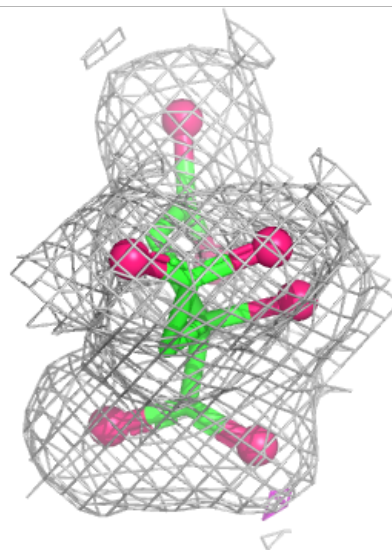
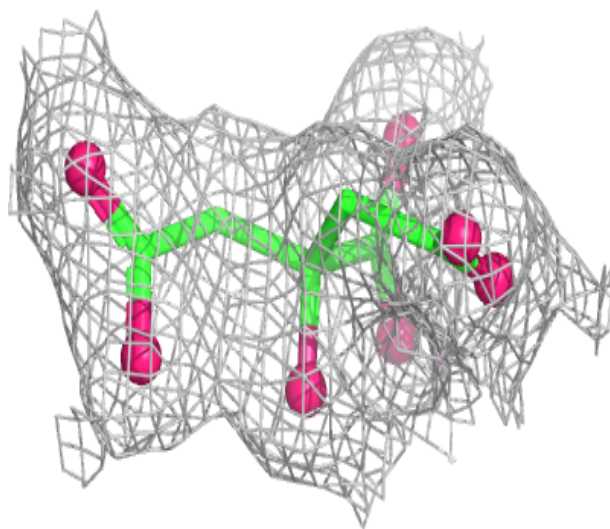
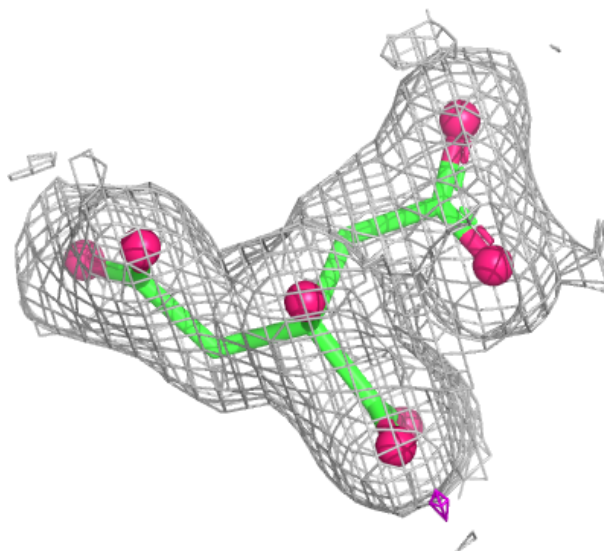
Electron density around CIT C 402:

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



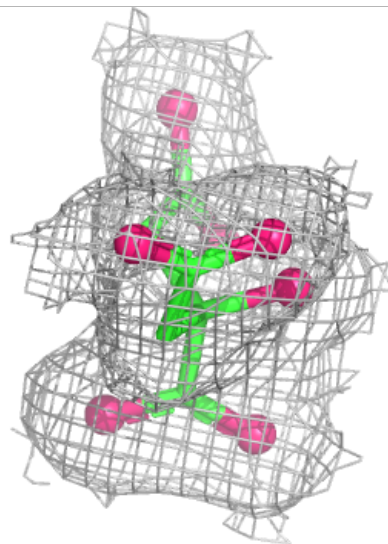
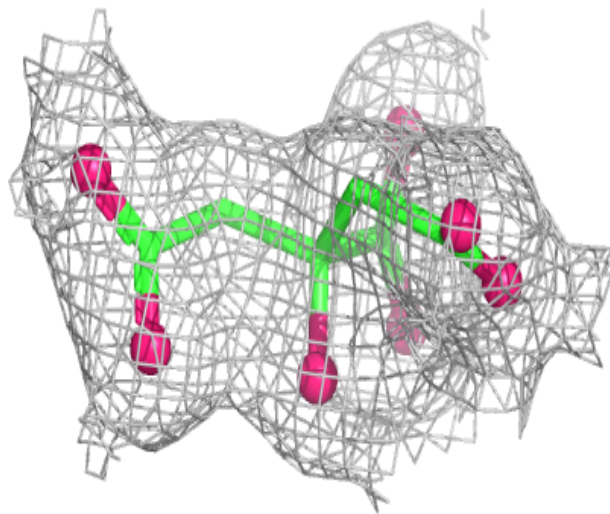
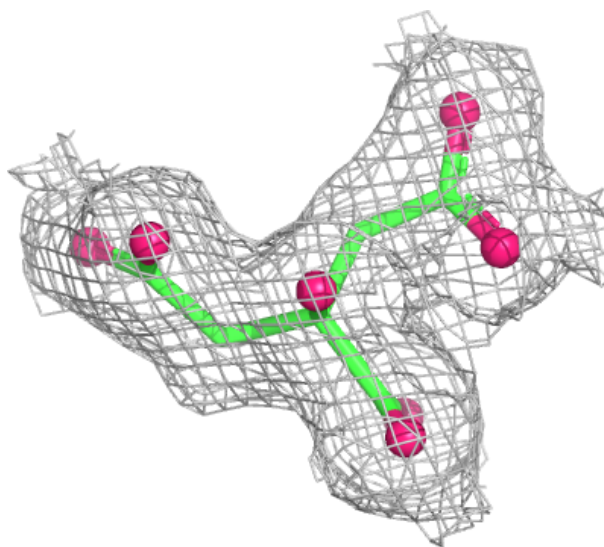
Electron density around CIT B 404:

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



Electron density around CIT A 403:

$2mF_o-DF_c$ (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.