wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 10:06 AM JST

PDB ID	:	6LNP
Title	:	Crystal structure of citrate Biosensor
Authors	:	Wen, Y.; Campbell, R.
Deposited on	:	2019-12-31
Resolution	:	2.99 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

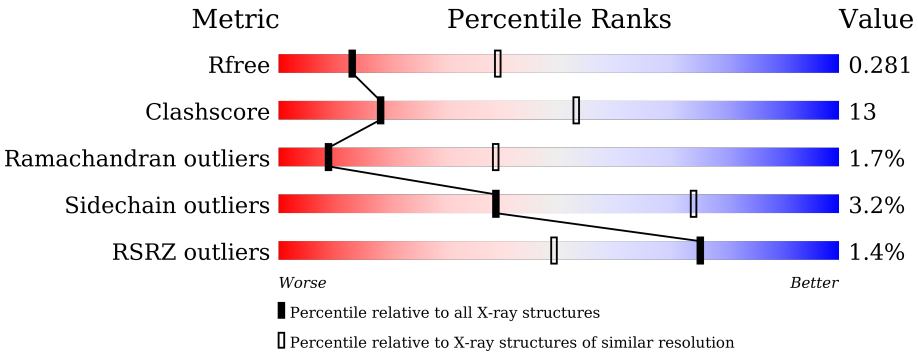
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	B	403	65% 26% • 8%
1	D	403	2% 66% 22% •• 10%

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
2	CIT	B	401	-	X	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5578 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 Fusion protein of Green fluorescent protein and Sensor histidine kinase CitA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	370	Total	C	N	O	S	0	0	0
			2796	1765	478	542	11			
1	D	363	Total	C	N	O	S	0	0	0
			2756	1738	477	530	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	112	VAL	-	linker	PDB ?
B	113	LYS	-	linker	PDB ?
B	114	PHE	-	linker	PDB ?
B	115	GLU	-	linker	PDB ?
B	116	GLY	-	linker	PDB ?
B	117	ASP	-	linker	PDB ?
B	118	THR	-	linker	PDB ?
B	119	LEU	-	linker	PDB ?
B	120	VAL	-	linker	PDB ?
B	121	ASN	-	linker	PDB ?
B	122	ARG	-	linker	PDB ?
B	123	ILE	-	linker	PDB ?
B	124	GLU	-	linker	PDB ?
B	125	LEU	-	linker	PDB ?
B	126	LYS	-	linker	PDB ?
B	127	GLY	-	linker	PDB ?
B	128	ALA	-	linker	PDB ?
B	129	ASP	-	linker	PDB ?
B	130	PHE	-	linker	PDB ?
B	131	ARG	-	linker	PDB ?
B	132	GLU	-	linker	PDB ?
B	133	ASP	-	linker	PDB ?
B	134	GLY	-	linker	PDB ?
B	135	ASN	-	linker	PDB ?

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Chain	Residue	Modelled	Actual	Comment	Reference
B	136	ILE	-	linker	PDB ?
B	137	LEU	-	linker	PDB ?
B	138	GLY	-	linker	PDB ?
B	139	HIS	-	linker	PDB ?
B	140	LYS	-	linker	PDB ?
B	141	LEU	-	linker	PDB ?
B	142	VAL	-	linker	PDB ?
B	143	TYR	-	linker	PDB ?
B	144	ASN	-	linker	PDB ?
B	145	MET	-	linker	PDB ?
B	146	VAL	-	linker	PDB ?
B	153	HIS	TYR	conflict	UNP P52687
B	168	THR	ALA	conflict	UNP P52687
B	195	PRO	SER	conflict	UNP P52687
B	223	VAL	GLU	conflict	UNP P52687
B	236	GLY	SER	conflict	UNP P52687
D	112	VAL	-	linker	PDB ?
D	113	LYS	-	linker	PDB ?
D	114	PHE	-	linker	PDB ?
D	115	GLU	-	linker	PDB ?
D	116	GLY	-	linker	PDB ?
D	117	ASP	-	linker	PDB ?
D	118	THR	-	linker	PDB ?
D	119	LEU	-	linker	PDB ?
D	120	VAL	-	linker	PDB ?
D	121	ASN	-	linker	PDB ?
D	122	ARG	-	linker	PDB ?
D	123	ILE	-	linker	PDB ?
D	124	GLU	-	linker	PDB ?
D	125	LEU	-	linker	PDB ?
D	126	LYS	-	linker	PDB ?
D	127	GLY	-	linker	PDB ?
D	128	ALA	-	linker	PDB ?
D	129	ASP	-	linker	PDB ?
D	130	PHE	-	linker	PDB ?
D	131	ARG	-	linker	PDB ?
D	132	GLU	-	linker	PDB ?
D	133	ASP	-	linker	PDB ?
D	134	GLY	-	linker	PDB ?
D	135	ASN	-	linker	PDB ?
D	136	ILE	-	linker	PDB ?
D	137	LEU	-	linker	PDB ?

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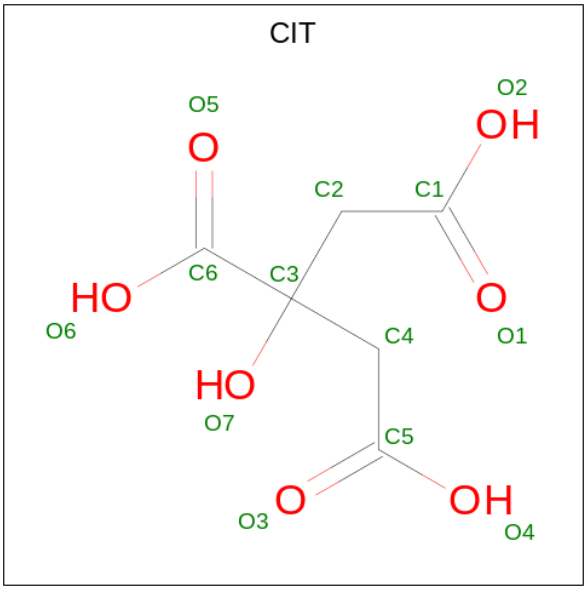
Chain	Residue	Modelled	Actual	Comment	Reference
D	138	GLY	-	linker	PDB ?
D	139	HIS	-	linker	PDB ?
D	140	LYS	-	linker	PDB ?
D	141	LEU	-	linker	PDB ?
D	142	VAL	-	linker	PDB ?
D	143	TYR	-	linker	PDB ?
D	144	ASN	-	linker	PDB ?
D	145	MET	-	linker	PDB ?
D	146	VAL	-	linker	PDB ?
D	153	HIS	TYR	conflict	UNP P52687
D	168	THR	ALA	conflict	UNP P52687
D	195	PRO	SER	conflict	UNP P52687
D	223	VAL	GLU	conflict	UNP P52687
D	236	GLY	SER	conflict	UNP P52687

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$) (labeled as "Ligand of Interest" by depositor).



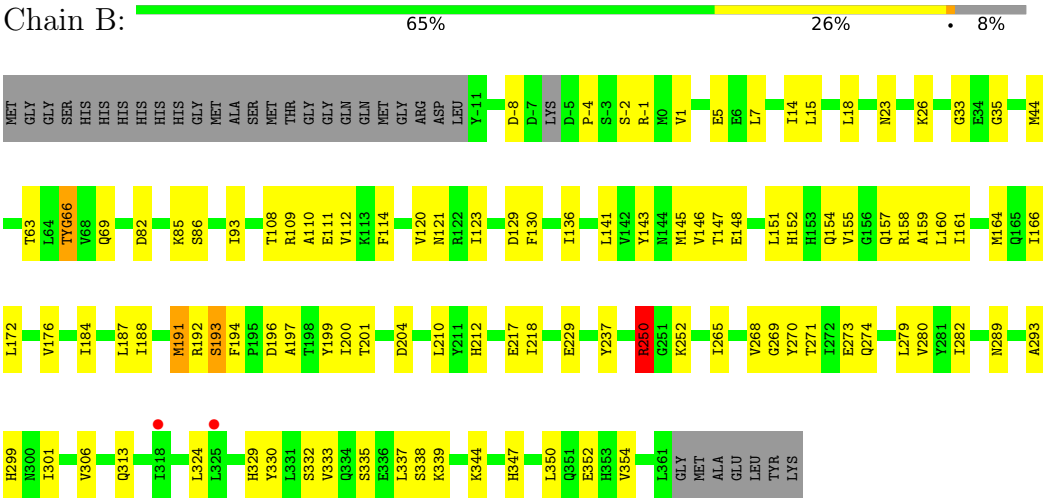
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0

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.

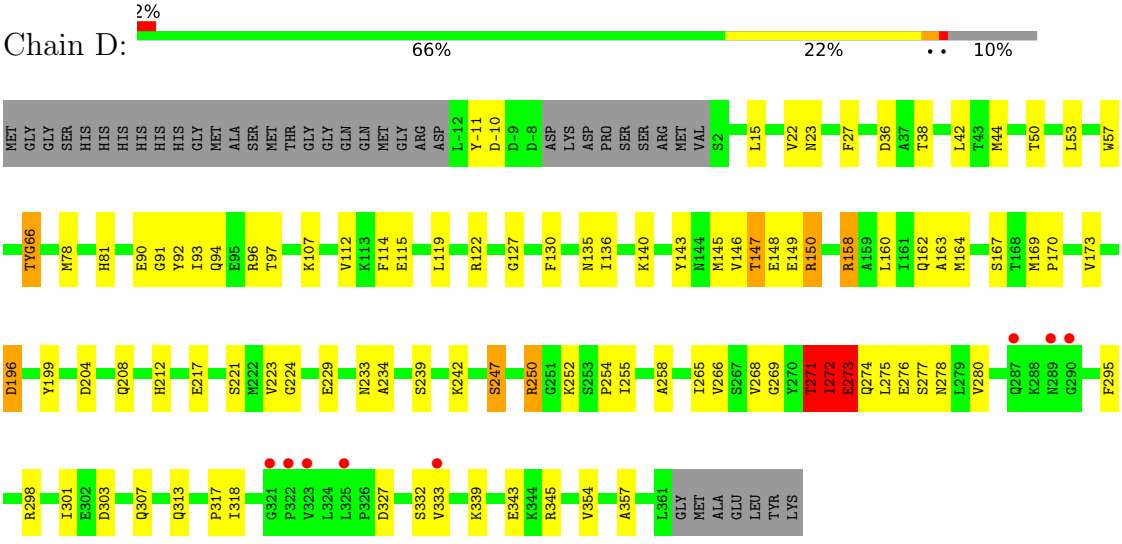
• Molecule 1: Fusion protein of Green fluorescent protein and Sensor histidine kinase CitA

Chain B:



• Molecule 1: Fusion protein of Green fluorescent protein and Sensor histidine kinase CitA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	92.41Å 92.41Å 123.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.20 – 2.99 46.21 – 2.99	Depositor EDS
% Data completeness (in resolution range)	85.4 (46.20-2.99) 85.4 (46.21-2.99)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.223 , 0.282 0.224 , 0.281	Depositor DCC
R_{free} test set	1793 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	5578	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CIT, CRO

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	B	0.34	1/2827 (0.0%)	0.52	1/3833 (0.0%)
1	D	0.34	0/2784	0.56	3/3770 (0.1%)
All	All	0.34	1/5611 (0.0%)	0.54	4/7603 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	250	ARG	C-O	-5.24	1.13	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	272	ILE	C-N-CA	7.08	139.39	121.70
1	D	273	GLU	N-CA-C	6.58	128.75	111.00
1	D	271	THR	N-CA-C	-6.52	93.39	111.00
1	B	250	ARG	NE-CZ-NH1	5.11	122.86	120.30

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	B	2796	0	2656	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2756	0	2650	74	0
2	B	13	0	5	1	0
2	D	13	0	5	1	0
All	All	5578	0	5316	146	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 13.

The worst 5 of 146 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:GLN:HB2	1:D:275:LEU:HD23	1.41	0.99
1:D:333:VAL:HG22	1:D:354:VAL:HG13	1.55	0.86
1:B:146:VAL:H	1:B:147:THR:HB	1.42	0.84
1:D:333:VAL:HG13	1:D:354:VAL:HG22	1.67	0.76
1:B:188:ILE:O	1:B:191:MET:HB2	1.89	0.72

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	B	363/403 (90%)	327 (90%)	30 (8%)	6 (2%)	9 39
1	D	356/403 (88%)	325 (91%)	25 (7%)	6 (2%)	9 39
All	All	719/806 (89%)	652 (91%)	55 (8%)	12 (2%)	9 39

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1	VAL

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Mol	Chain	Res	Type
1	D	-10	ASP
1	D	147	THR
1	D	272	ILE
1	D	273	GLU

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	B	285/338 (84%)	277 (97%)	8 (3%)	43 77
1	D	285/338 (84%)	275 (96%)	10 (4%)	36 71
All	All	570/676 (84%)	552 (97%)	18 (3%)	39 74

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	247	SER
1	D	332	SER
1	D	271	THR
1	D	-11	TYR
1	D	239	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	212	HIS
1	D	212	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CRO	D	66	1	23,23,24	3.09	5 (21%)	30,32,34	3.18	8 (26%)
1	CRO	B	66	1	23,23,24	3.11	7 (30%)	30,32,34	3.07	6 (20%)

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
1	CRO	D	66	1	-	1/12/31/32	0/2/2/2
1	CRO	B	66	1	-	5/12/31/32	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRO	CA2-C2	-12.61	1.36	1.48
1	D	66	CRO	CA2-C2	-12.49	1.36	1.48
1	B	66	CRO	C2-N3	-3.64	1.31	1.39
1	D	66	CRO	C2-N3	-3.60	1.31	1.39
1	D	66	CRO	CB2-CA2	-3.56	1.32	1.35

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	66	CRO	CA2-C2-N3	11.27	108.70	103.37
1	B	66	CRO	CA2-C2-N3	10.79	108.47	103.37
1	B	66	CRO	O2-C2-CA2	-9.83	125.44	130.96
1	D	66	CRO	O2-C2-CA2	-9.53	125.61	130.96
1	D	66	CRO	N3-C1-N2	-5.84	107.41	111.45

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	66	CRO	N1-CA1-CB1-CG1
1	B	66	CRO	C1-CA1-CB1-CG1
1	B	66	CRO	C1-CA1-CB1-OG1
1	D	66	CRO	C2-CA2-CB2-CG2
1	B	66	CRO	C3-CA3-N3-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	66	CRO	2	0
1	B	66	CRO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	D	401	-	12,12,12	1.06	0	17,17,17	1.45	1 (5%)
2	CIT	B	401	-	12,12,12	2.07	6 (50%)	17,17,17	2.06	4 (23%)

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	D	401	-	-	9/16/16/16	-
2	CIT	B	401	-	-	13/16/16/16	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	CIT	C3-C6	-3.53	1.49	1.53
2	B	401	CIT	C2-C3	-3.37	1.49	1.53
2	B	401	CIT	O4-C5	-3.28	1.19	1.30
2	B	401	CIT	O7-C3	-2.52	1.38	1.43
2	B	401	CIT	O6-C6	-2.22	1.22	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	CIT	O6-C6-C3	4.75	121.30	113.05
2	B	401	CIT	C4-C3-C6	4.07	118.84	110.11
2	D	401	CIT	O6-C6-C3	3.99	119.99	113.05
2	B	401	CIT	C3-C4-C5	3.02	121.13	113.81
2	B	401	CIT	O7-C3-C6	-2.48	105.38	108.86

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	CIT	O7-C3-C6-O5
2	B	401	CIT	O7-C3-C6-O6
2	B	401	CIT	C4-C3-C6-O5
2	B	401	CIT	C4-C3-C6-O6
2	D	401	CIT	O7-C3-C6-O5

There are no ring outliers.

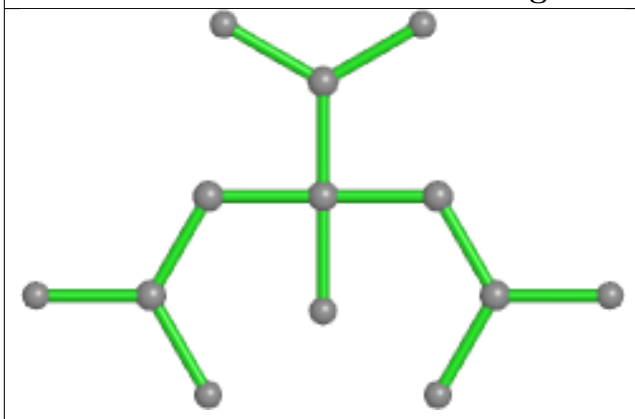
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	CIT	1	0
2	B	401	CIT	1	0

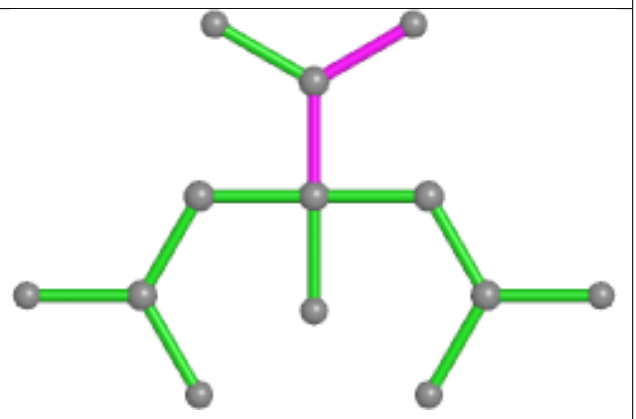
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

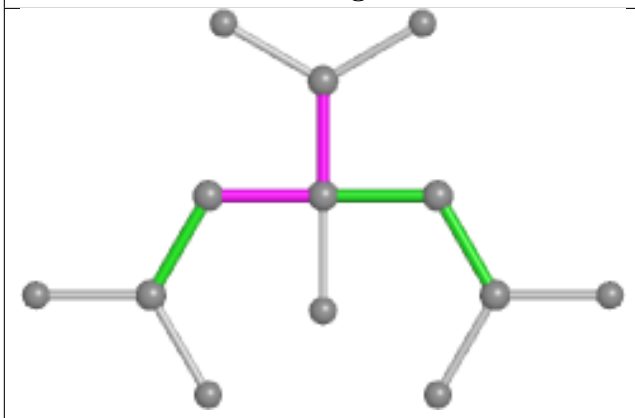
Ligand CIT D 401



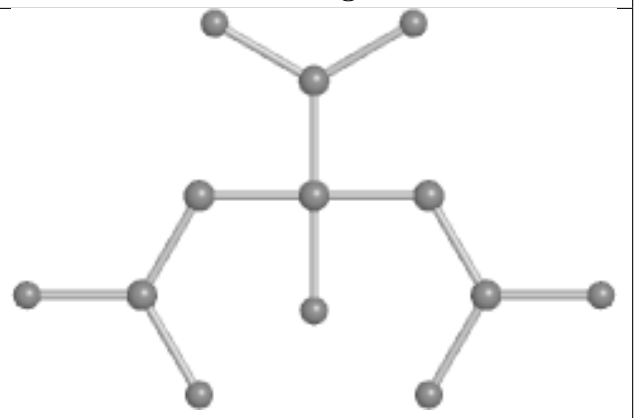
Bond lengths



Bond angles

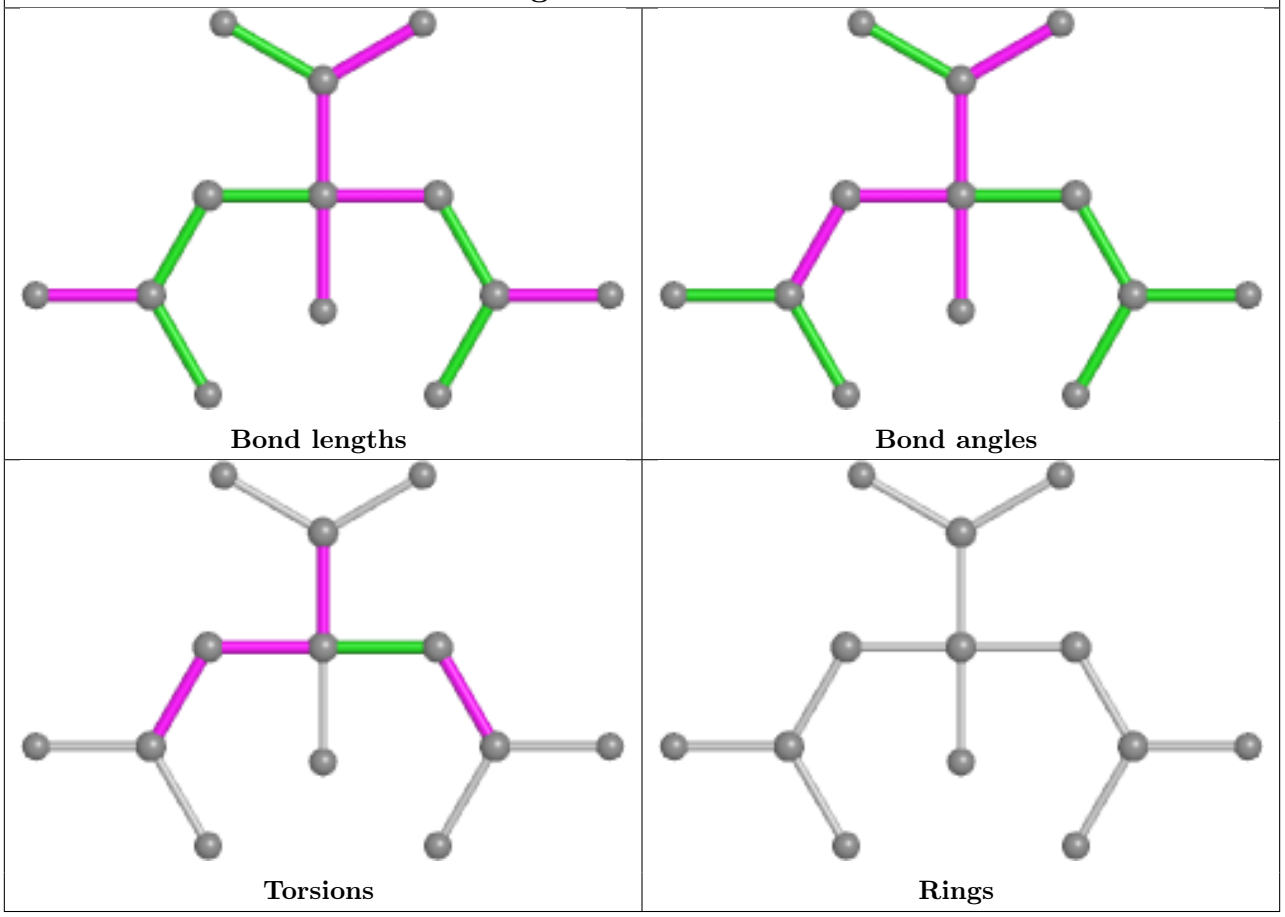


Torsions



Rings

Ligand CIT B 401



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^{th} 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	B	369/403 (91%)	0.06	2 (0%)	91	75	19, 49, 89, 127	0
1	D	362/403 (89%)	0.04	8 (2%)	62	33	23, 46, 78, 123	0
All	All	731/806 (90%)	0.05	10 (1%)	75	49	19, 48, 84, 127	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318	ILE	3.2
1	D	290	GLY	3.2
1	D	325	LEU	3.0
1	D	322	PRO	2.9
1	B	325	LEU	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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^{th} 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
1	CRO	B	66	22/23	0.94	0.23	55,60,63,65	0
1	CRO	D	66	22/23	0.94	0.22	50,50,52,53	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

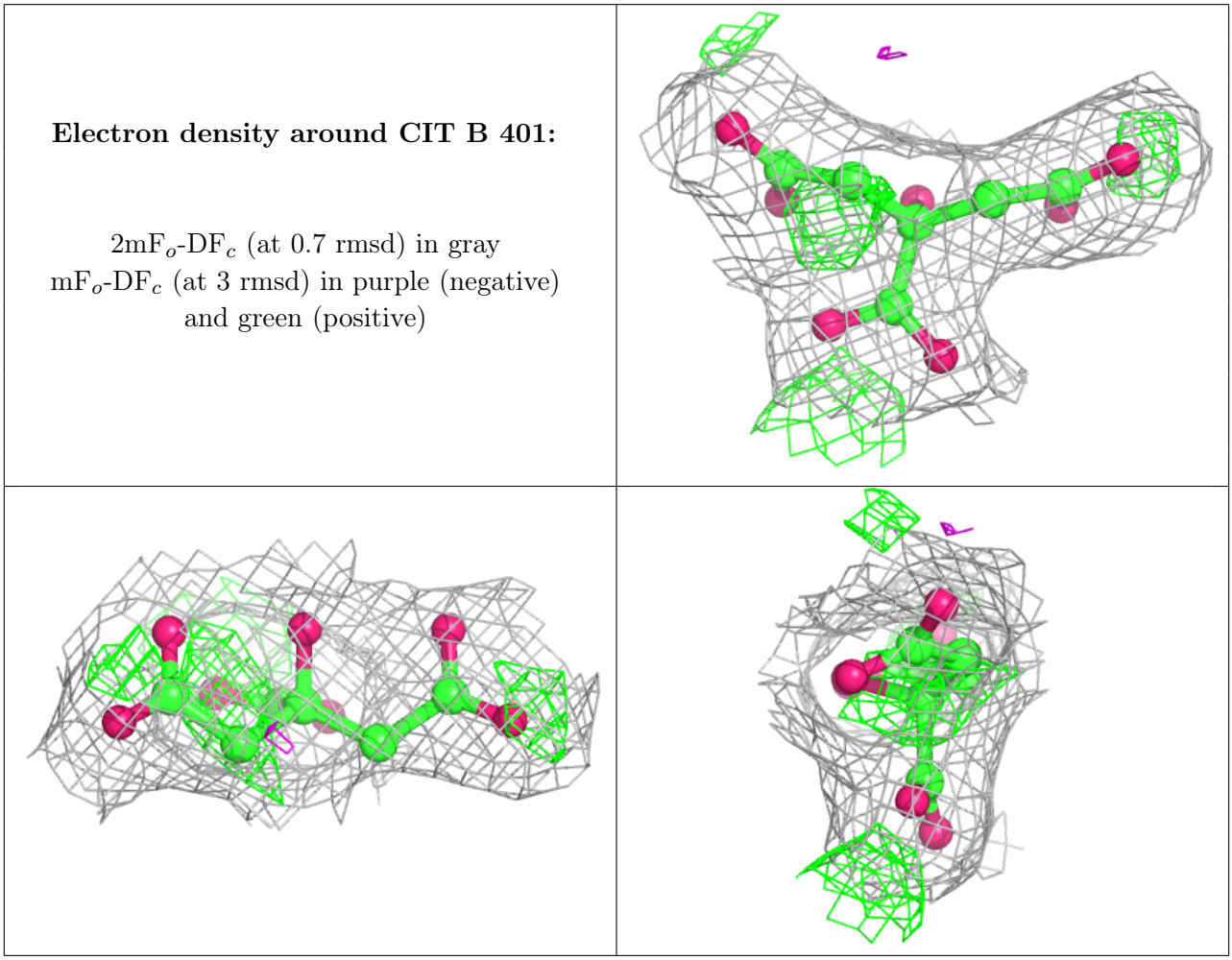
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	CIT	B	401	13/13	0.90	0.19	53,54,54,55	0
2	CIT	D	401	13/13	0.93	0.18	49,50,51,51	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.

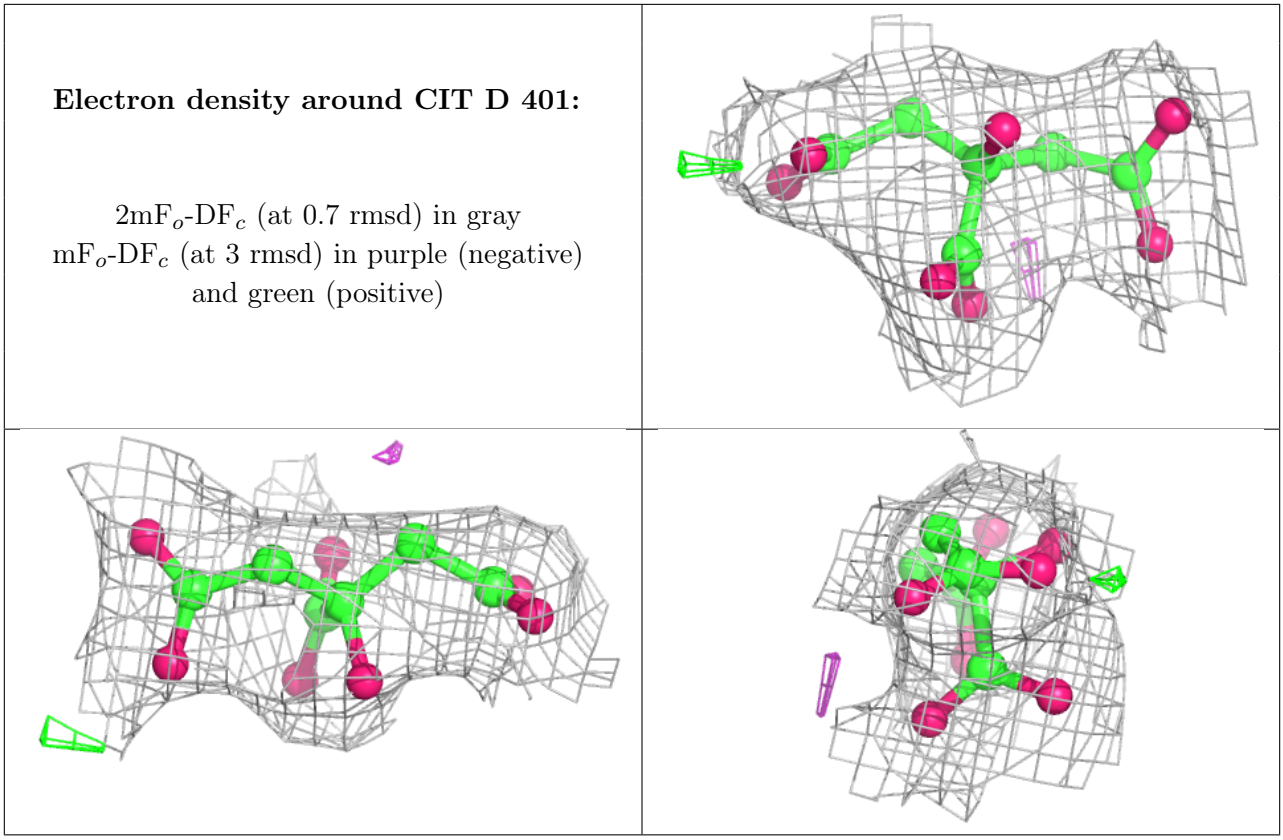
Electron density around CIT B 401:

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



Electron density around CIT D 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

There are no such residues in this entry.