Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 12:31 AM JST

PDB ID	:	7E2W
Title	:	Crystal structure of isocitrate dehydrogenase from Ostreococcus tauri in complex with isocitrate and magnesium(II)
Authors	:	Zhu, G.P.; Tang, W.G.; Wang, P.
Deposited on	:	2021-02-07
Resolution	:	1.80 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:

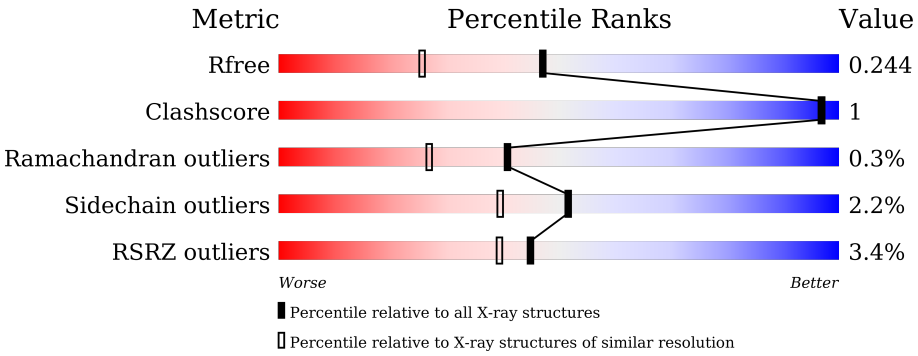
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	A	418	94%
1	B	418	2% 92% 5%
1	C	418	7% 89% 6%
1	D	418	3% 92% 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13038 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 Isocitrate dehydrogenase (NAD(+)), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3131	1977	555	585	14			
1	B	404	Total	C	N	O	S	0	0	0
			3109	1962	543	590	14			
1	C	400	Total	C	N	O	S	0	0	0
			3000	1902	518	566	14			
1	D	396	Total	C	N	O	S	0	0	0
			3048	1925	537	572	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP A0A096P8D3
A	13	HIS	-	expression tag	UNP A0A096P8D3
A	14	HIS	-	expression tag	UNP A0A096P8D3
A	15	HIS	-	expression tag	UNP A0A096P8D3
A	16	HIS	-	expression tag	UNP A0A096P8D3
A	17	HIS	-	expression tag	UNP A0A096P8D3
A	18	HIS	-	expression tag	UNP A0A096P8D3
A	19	HIS	-	expression tag	UNP A0A096P8D3
B	12	GLY	-	expression tag	UNP A0A096P8D3
B	13	HIS	-	expression tag	UNP A0A096P8D3
B	14	HIS	-	expression tag	UNP A0A096P8D3
B	15	HIS	-	expression tag	UNP A0A096P8D3
B	16	HIS	-	expression tag	UNP A0A096P8D3
B	17	HIS	-	expression tag	UNP A0A096P8D3
B	18	HIS	-	expression tag	UNP A0A096P8D3
B	19	HIS	-	expression tag	UNP A0A096P8D3
C	12	GLY	-	expression tag	UNP A0A096P8D3
C	13	HIS	-	expression tag	UNP A0A096P8D3
C	14	HIS	-	expression tag	UNP A0A096P8D3
C	15	HIS	-	expression tag	UNP A0A096P8D3
C	16	HIS	-	expression tag	UNP A0A096P8D3

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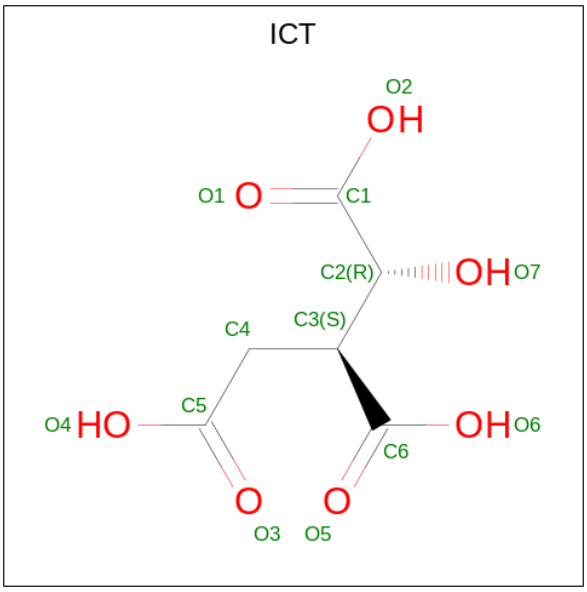
Chain	Residue	Modelled	Actual	Comment	Reference
C	17	HIS	-	expression tag	UNP A0A096P8D3
C	18	HIS	-	expression tag	UNP A0A096P8D3
C	19	HIS	-	expression tag	UNP A0A096P8D3
D	12	GLY	-	expression tag	UNP A0A096P8D3
D	13	HIS	-	expression tag	UNP A0A096P8D3
D	14	HIS	-	expression tag	UNP A0A096P8D3
D	15	HIS	-	expression tag	UNP A0A096P8D3
D	16	HIS	-	expression tag	UNP A0A096P8D3
D	17	HIS	-	expression tag	UNP A0A096P8D3
D	18	HIS	-	expression tag	UNP A0A096P8D3
D	19	HIS	-	expression tag	UNP A0A096P8D3

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

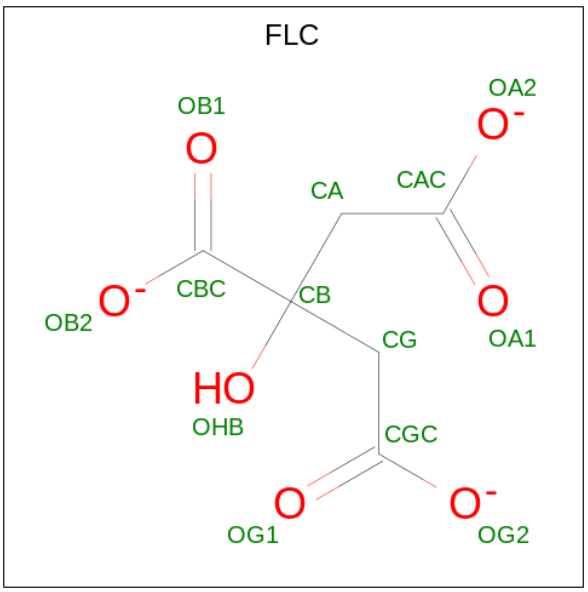


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

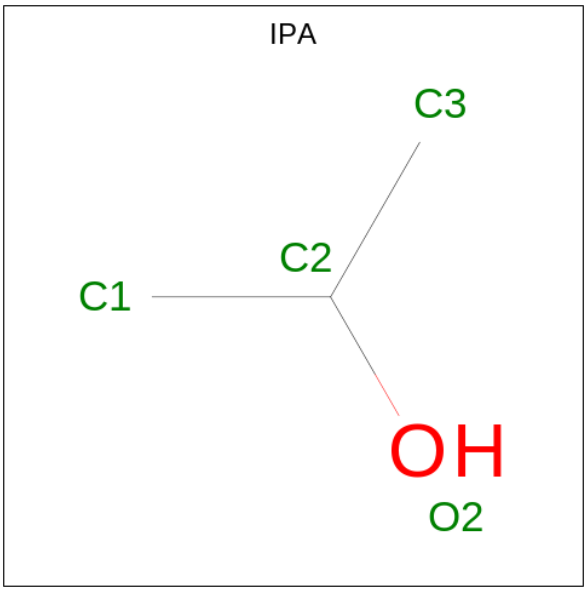
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



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

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



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

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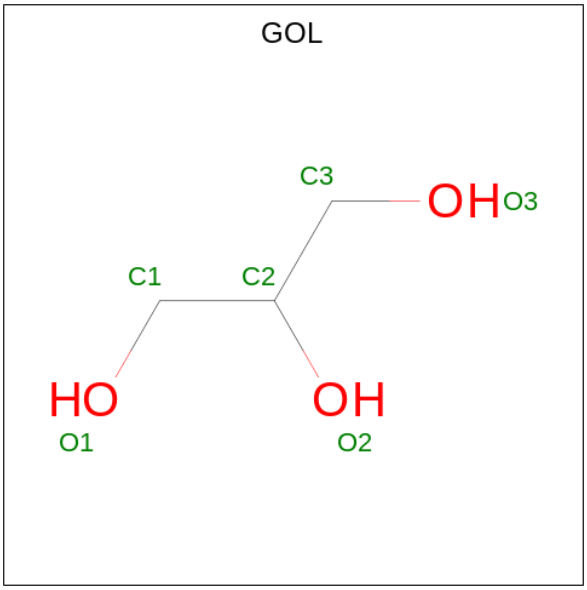
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 3 1	0	0

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



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

- Molecule 7 is water.

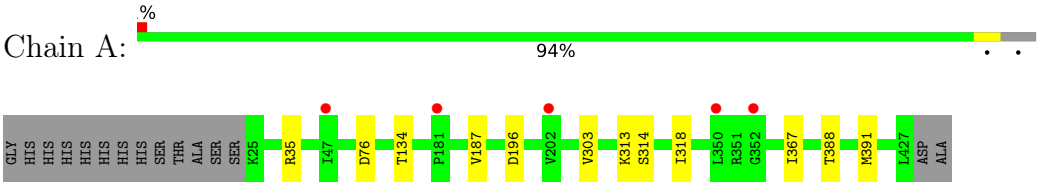
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	165	Total O 165 165	0	0
7	B	196	Total O 196 196	0	0
7	C	128	Total O 128 128	0	0
7	D	204	Total O 204 204	0	0

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.

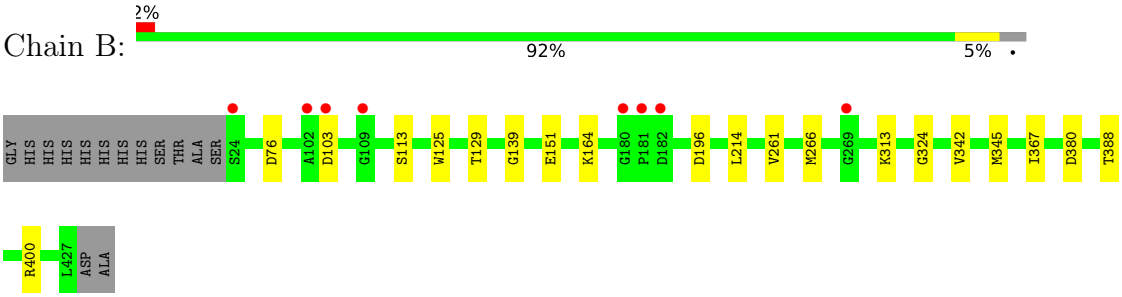
• Molecule 1: Isocitrate dehydrogenase (NAD(+)), mitochondrial

Chain A:



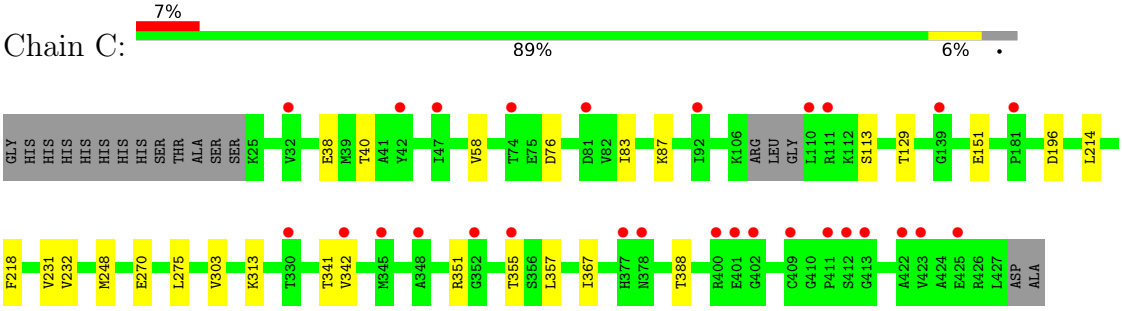
• Molecule 1: Isocitrate dehydrogenase (NAD(+)), mitochondrial

Chain B:



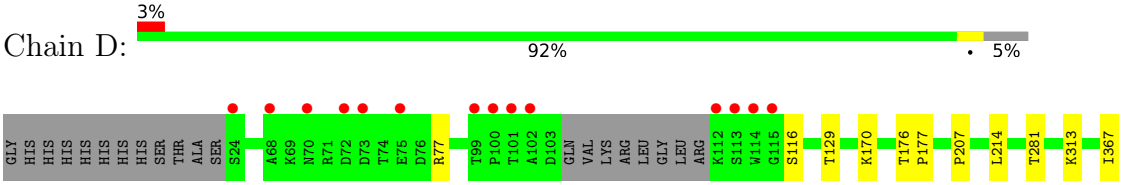
• Molecule 1: Isocitrate dehydrogenase (NAD(+)), mitochondrial

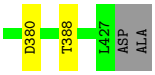
Chain C:



• Molecule 1: Isocitrate dehydrogenase (NAD(+)), mitochondrial

Chain D:




D380
T388
L427
ASP
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.25Å 78.51Å 111.06Å 89.15° 103.59° 111.89°	Depositor
Resolution (Å)	19.95 – 1.80 19.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.9 (19.95-1.80) 95.0 (19.94-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.208 , 0.239 0.215 , 0.244	Depositor DCC
R_{free} test set	8824 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13038	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: MG, GOL, ICT, IPA, FLC

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	0.71	0/3198	0.82	0/4333
1	B	0.70	0/3176	0.83	0/4310
1	C	0.63	0/3066	0.81	0/4167
1	D	0.68	0/3112	0.79	0/4214
All	All	0.68	0/12552	0.81	0/17024

There are no bond length outliers.

There are no bond angle outliers.

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	3131	0	3036	3	0
1	B	3109	0	2981	8	0
1	C	3000	0	2816	8	0
1	D	3048	0	2949	4	0
2	A	13	0	4	0	0
3	A	1	0	0	0	0
4	A	13	0	5	0	0
5	A	4	0	8	0	0
5	C	4	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	4	0	8	0	0
6	C	6	0	8	0	0
6	D	12	0	16	0	0
7	A	165	0	0	0	0
7	B	196	0	0	0	0
7	C	128	0	0	0	0
7	D	204	0	0	0	0
All	All	13038	0	11839	21	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 1.

All (21) 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:367:ILE:HG23	1:D:388:THR:HB	1.87	0.57
1:B:367:ILE:HG23	1:B:388:THR:HB	1.87	0.57
1:C:303:VAL:HG13	1:D:281:THR:HG21	1.88	0.56
1:D:129:THR:HB	1:D:214:LEU:HD13	1.89	0.54
1:B:139:GLY:HA3	1:B:400:ARG:HD3	1.90	0.52
1:C:129:THR:HB	1:C:214:LEU:HD13	1.92	0.52
1:A:367:ILE:HG23	1:A:388:THR:HB	1.92	0.52
1:C:367:ILE:HG23	1:C:388:THR:HB	1.92	0.52
1:B:261:VAL:HA	1:B:266:MET:O	2.15	0.47
1:A:134:THR:HA	1:A:318:ILE:HD13	1.97	0.46
1:C:151:GLU:HG3	1:C:218:PHE:CD1	2.51	0.46
1:C:40:THR:OG1	1:C:341:THR:HA	2.18	0.44
1:B:129:THR:HB	1:B:214:LEU:CD1	2.48	0.43
1:A:187:VAL:HG21	1:B:164:LYS:HE2	2.01	0.42
1:B:129:THR:HB	1:B:214:LEU:HD13	2.01	0.42
1:C:38:GLU:HB2	1:C:341:THR:HB	2.02	0.42
1:D:176:THR:HA	1:D:177:PRO:HD2	1.93	0.41
1:B:342:VAL:HG12	1:B:345:MET:HB2	2.02	0.41
1:C:232:VAL:HA	1:C:275:LEU:O	2.21	0.41
1:B:125:TRP:O	1:B:324:GLY:HA3	2.21	0.40
1:C:231:VAL:HG22	1:C:248:MET:HE2	2.02	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	401/418 (96%)	390 (97%)	10 (2%)	1 (0%)	47	33
1	B	402/418 (96%)	393 (98%)	8 (2%)	1 (0%)	47	33
1	C	396/418 (95%)	378 (96%)	16 (4%)	2 (0%)	29	15
1	D	392/418 (94%)	376 (96%)	15 (4%)	1 (0%)	41	27
All	All	1591/1672 (95%)	1537 (97%)	49 (3%)	5 (0%)	41	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	LYS
1	B	313	LYS
1	C	313	LYS
1	D	313	LYS
1	C	58	VAL

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	319/346 (92%)	313 (98%)	6 (2%)	57	46
1	B	316/346 (91%)	310 (98%)	6 (2%)	57	46
1	C	292/346 (84%)	282 (97%)	10 (3%)	37	22
1	D	310/346 (90%)	305 (98%)	5 (2%)	62	54
All	All	1237/1384 (89%)	1210 (98%)	27 (2%)	52	39

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	76	ASP
1	A	196	ASP
1	A	303	VAL
1	A	314	SER
1	A	391	MET
1	B	76	ASP
1	B	103	ASP
1	B	113	SER
1	B	151	GLU
1	B	196	ASP
1	B	380	ASP
1	C	76	ASP
1	C	83	ILE
1	C	87	LYS
1	C	113	SER
1	C	196	ASP
1	C	270	GLU
1	C	342	VAL
1	C	351	ARG
1	C	355	THR
1	C	357	LEU
1	D	77	ARG
1	D	116	SER
1	D	170	LYS
1	D	207	PRO
1	D	380	ASP

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
6	GOL	D	500	-	5,5,5	0.19	0	5,5,5	0.40	0
5	IPA	C	501	-	3,3,3	0.44	0	3,3,3	0.23	0
2	ICT	A	500	3	12,12,12	1.26	0	13,16,16	1.26	1 (7%)
4	FLC	A	502	-	12,12,12	1.04	0	17,17,17	1.13	1 (5%)
6	GOL	D	501	-	5,5,5	0.17	0	5,5,5	0.47	0
5	IPA	A	503	-	3,3,3	0.33	0	3,3,3	0.13	0
6	GOL	C	500	-	5,5,5	0.17	0	5,5,5	0.34	0
5	IPA	D	502	-	3,3,3	0.32	0	3,3,3	0.11	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
6	GOL	D	500	-	-	2/4/4/4	-
2	ICT	A	500	3	-	4/16/16/16	-
4	FLC	A	502	-	-	5/16/16/16	-
6	GOL	D	501	-	-	4/4/4/4	-
6	GOL	C	500	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	FLC	OB1-CBC-CB	-2.72	118.41	122.25
2	A	500	ICT	O7-C2-C3	-2.14	105.38	110.58

There are no chirality outliers.

All (19) torsion outliers are listed below:

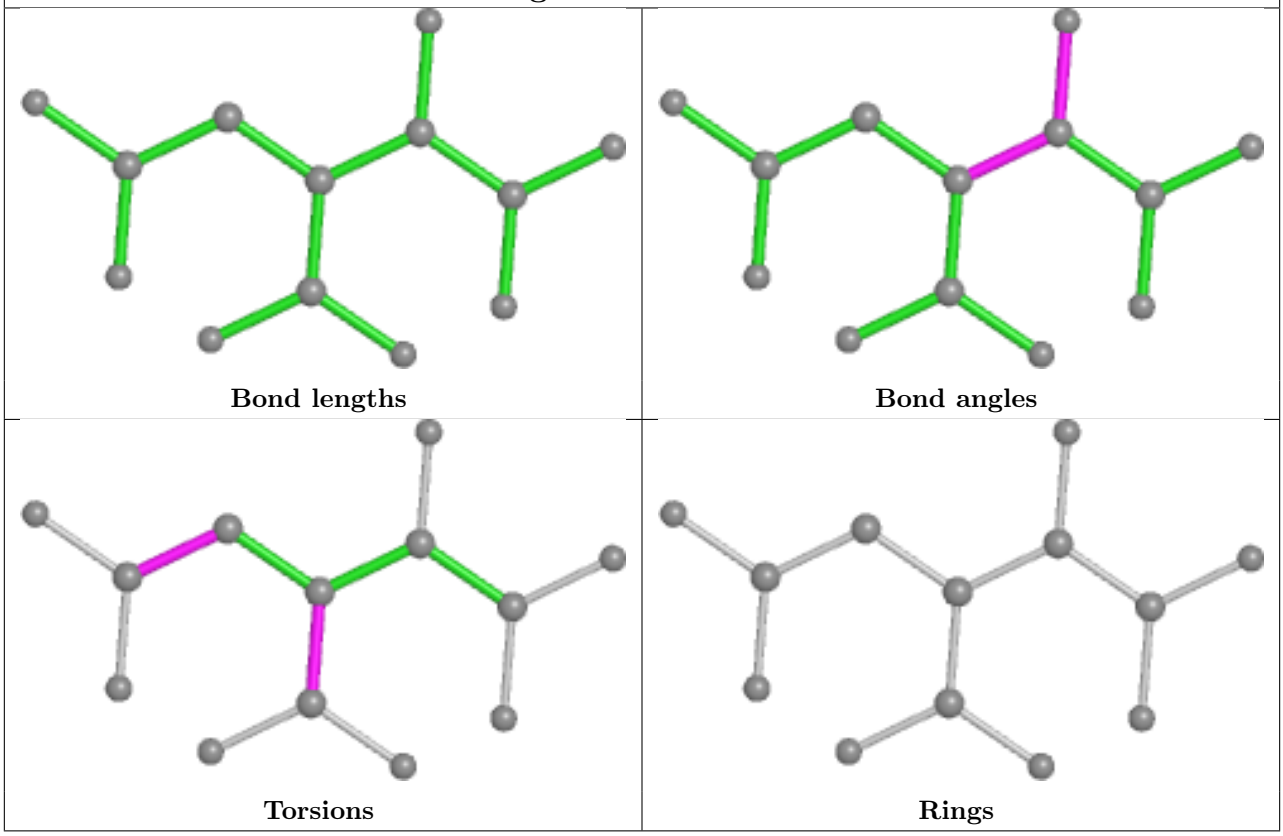
Mol	Chain	Res	Type	Atoms
4	A	502	FLC	CA-CB-CG-CGC
4	A	502	FLC	CBC-CB-CG-CGC
4	A	502	FLC	OHB-CB-CG-CGC
6	C	500	GOL	C1-C2-C3-O3
6	D	501	GOL	O1-C1-C2-C3
6	D	501	GOL	C1-C2-C3-O3
6	C	500	GOL	O1-C1-C2-C3
6	D	500	GOL	C1-C2-C3-O3
6	C	500	GOL	O1-C1-C2-O2
6	C	500	GOL	O2-C2-C3-O3
6	D	501	GOL	O1-C1-C2-O2
2	A	500	ICT	C4-C3-C6-O6
6	D	501	GOL	O2-C2-C3-O3
4	A	502	FLC	CAC-CA-CB-CG
2	A	500	ICT	C4-C3-C6-O5
6	D	500	GOL	O2-C2-C3-O3
4	A	502	FLC	CAC-CA-CB-CBC
2	A	500	ICT	C3-C4-C5-O4
2	A	500	ICT	C3-C4-C5-O3

There are no ring outliers.

No monomer is involved in short contacts.

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 ICT A 500



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	A	403/418 (96%)	-0.20	5 (1%)	79	76	16, 29, 47, 60	0
1	B	404/418 (96%)	-0.17	8 (1%)	65	61	20, 29, 51, 63	0
1	C	400/418 (95%)	0.40	28 (7%)	16	13	17, 37, 64, 88	0
1	D	396/418 (94%)	-0.12	14 (3%)	44	38	16, 27, 56, 72	0
All	All	1603/1672 (95%)	-0.02	55 (3%)	45	39	16, 29, 57, 88	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	413	GLY	6.2
1	C	411	PRO	4.6
1	A	350	LEU	4.3
1	D	102	ALA	4.2
1	D	100	PRO	4.2
1	C	425	GLU	4.2
1	C	422	ALA	4.1
1	D	113	SER	4.1
1	C	81	ASP	3.9
1	C	355	THR	3.8
1	C	412	SER	3.8
1	D	114	TRP	3.6
1	C	378	ASN	3.6
1	C	352	GLY	3.4
1	B	269	GLY	3.3
1	C	402	GLY	3.2
1	C	342	VAL	3.2
1	A	352	GLY	3.2
1	A	181	PRO	3.0
1	C	400	ARG	3.0
1	B	180	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	181	PRO	2.7
1	C	32	VAL	2.6
1	D	73	ASP	2.6
1	D	24	SER	2.6
1	C	74	THR	2.6
1	B	102	ALA	2.6
1	C	181	PRO	2.5
1	D	99	THR	2.5
1	C	47	ILE	2.5
1	C	348	ALA	2.5
1	C	409	CYS	2.4
1	D	75	GLU	2.4
1	C	377	HIS	2.3
1	A	47	ILE	2.3
1	C	92	ILE	2.3
1	B	24	SER	2.3
1	C	139	GLY	2.3
1	D	68	ALA	2.3
1	D	112	LYS	2.2
1	A	202	VAL	2.2
1	C	423	VAL	2.2
1	D	115	GLY	2.2
1	D	101	THR	2.2
1	C	111	ARG	2.1
1	D	70	ASN	2.1
1	D	72	ASP	2.1
1	B	103	ASP	2.1
1	B	182	ASP	2.1
1	C	330	THR	2.1
1	C	401	GLU	2.1
1	C	42	TYR	2.1
1	B	109	GLY	2.1
1	C	110	LEU	2.0
1	C	345	MET	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)

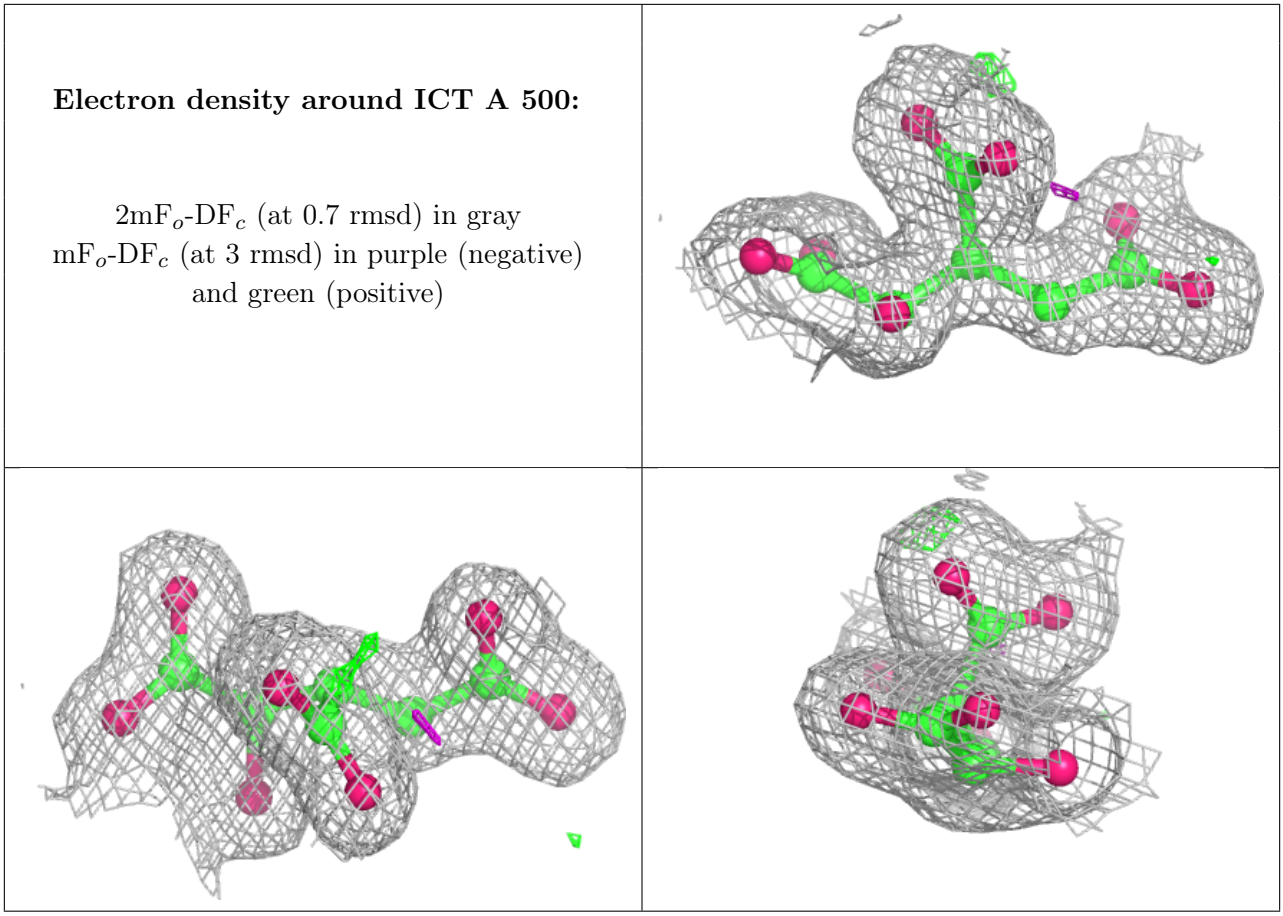
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	GOL	C	500	6/6	0.75	0.14	45,54,54,55	0
4	FLC	A	502	13/13	0.83	0.21	32,41,64,74	0
6	GOL	D	500	6/6	0.87	0.15	38,42,45,48	0
6	GOL	D	501	6/6	0.92	0.15	28,36,36,50	0
5	IPA	D	502	4/4	0.93	0.10	38,40,42,44	0
5	IPA	A	503	4/4	0.93	0.10	34,38,38,41	0
2	ICT	A	500	13/13	0.94	0.09	23,27,33,33	0
5	IPA	C	501	4/4	0.95	0.08	31,37,37,41	0
3	MG	A	501	1/1	0.99	0.02	26,26,26,26	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.

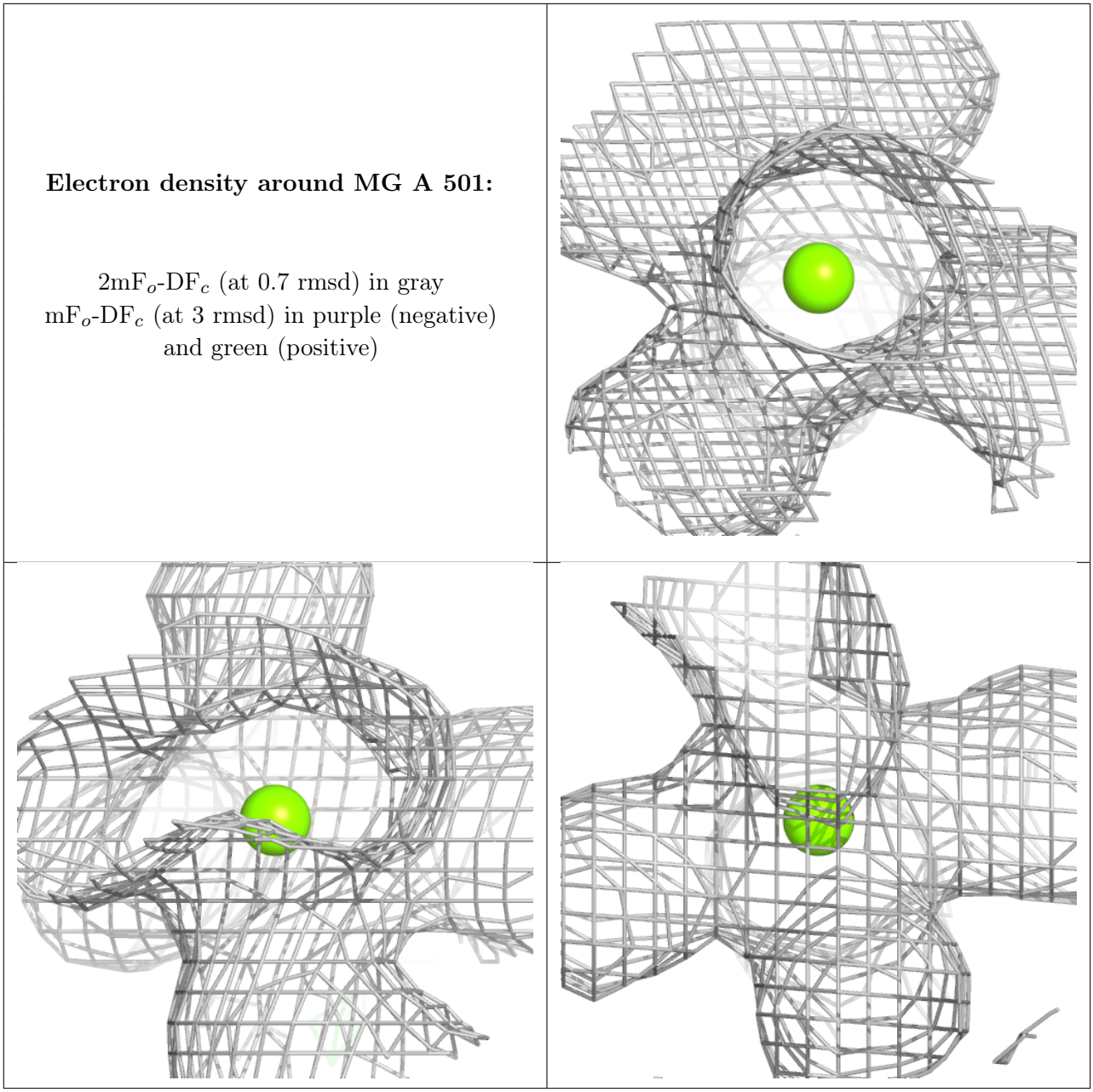
Electron density around ICT A 500:

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



Electron density around MG A 501:

$2mF_o$-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.