



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:48 AM UTC

PDB ID : 7E2W / pdb_00007e2w
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	:	4-5-2 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

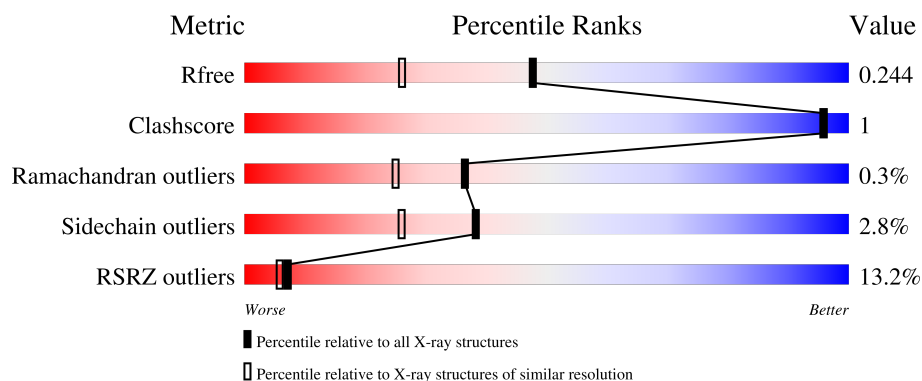
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 $\leq 5\%$. 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	418	4% 91% 5% .
1	B	418	5% 90% 7% .
1	C	418	33% 88% 7% .
1	D	418	9% 90% 5% 5%

2 Entry composition

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:

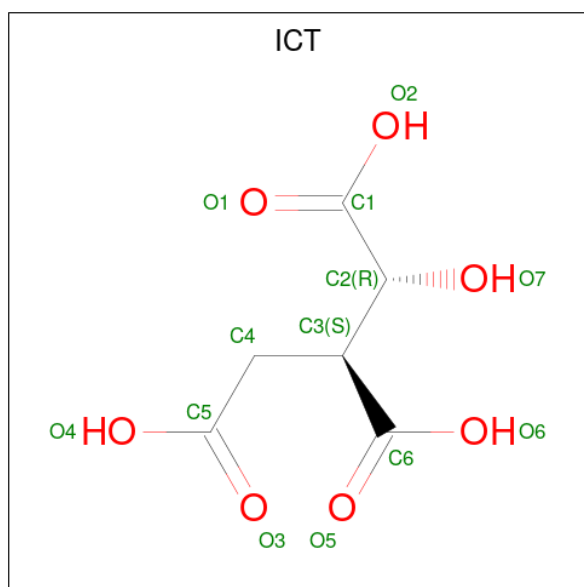
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP A0A096P8D3
A	13	HIS	-	expression tag	UNP A0A096P8D3
A	14	HIS	-	expression tag	UNP A0A096P8D3
A	15	HIS	-	expression tag	UNP A0A096P8D3
A	16	HIS	-	expression tag	UNP A0A096P8D3
A	17	HIS	-	expression tag	UNP A0A096P8D3
A	18	HIS	-	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 (CCD ID: ICT) (formula: $C_6H_8O_7$) (labeled as "Ligand of Interest" by depositor).

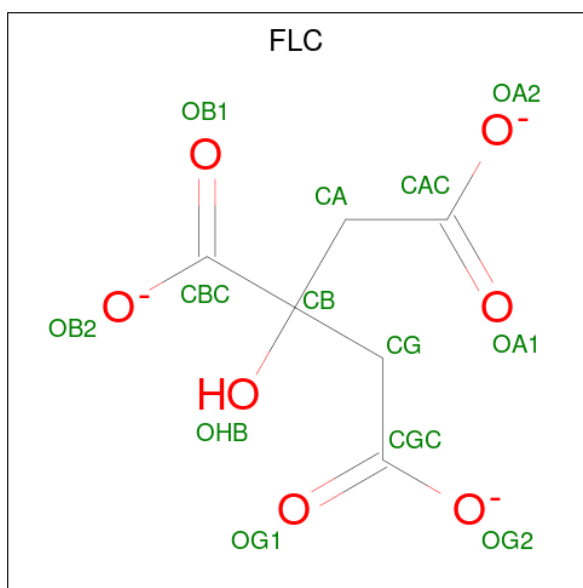


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

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

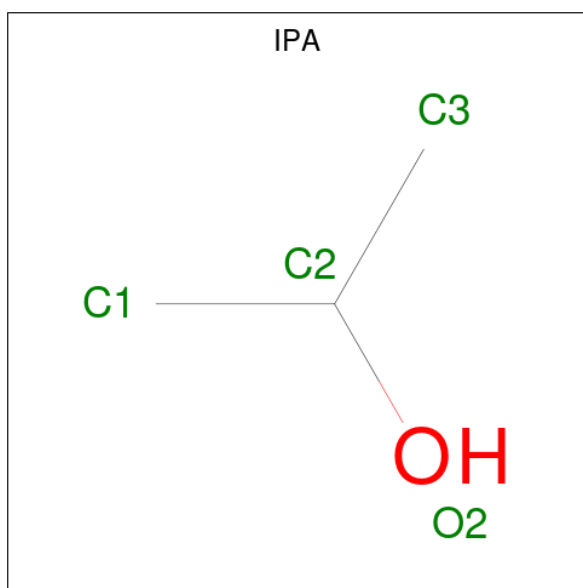
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



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

- Molecule 5 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



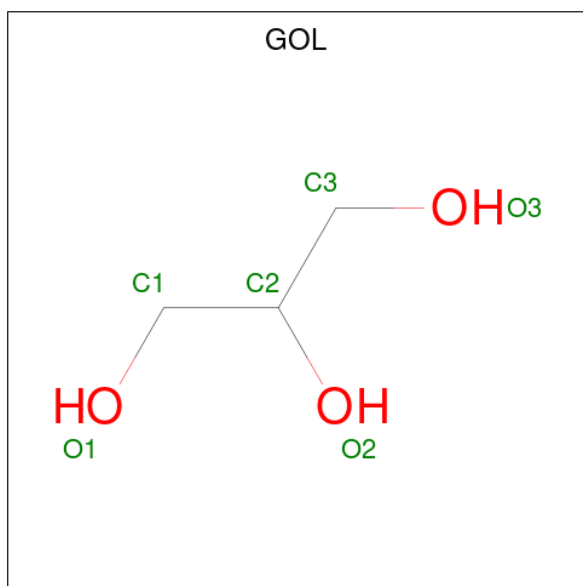
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	3	1		
5	C	1	Total	C	O	0	0
			4	3	1		

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

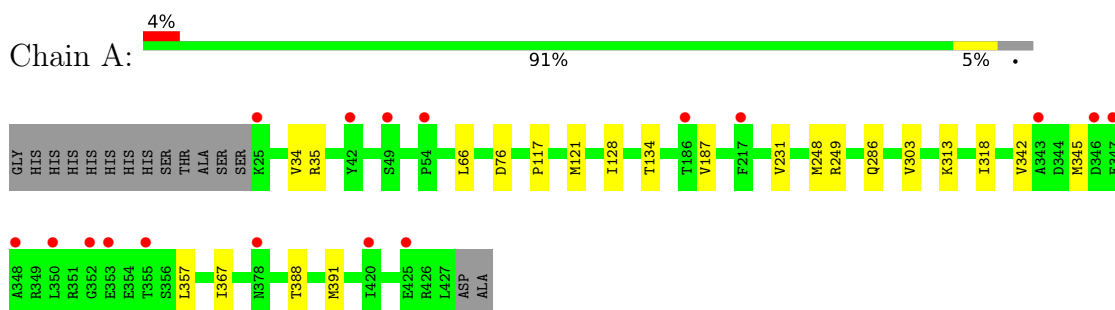
- Molecule 7 is water.

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

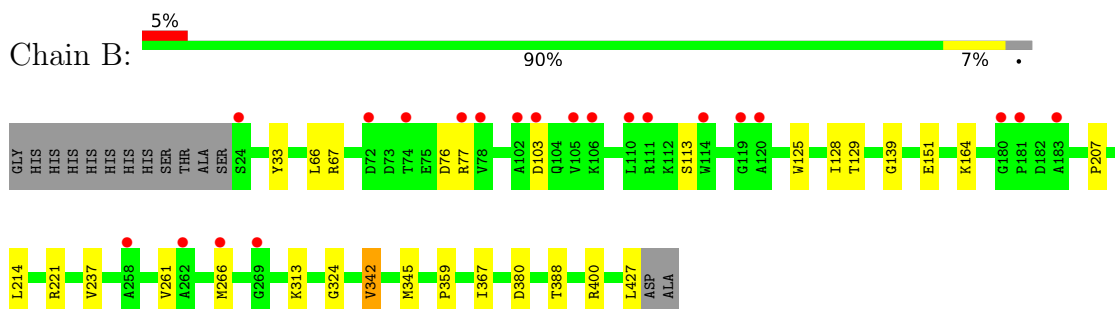
3 Residue-property plots [i](#)

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.

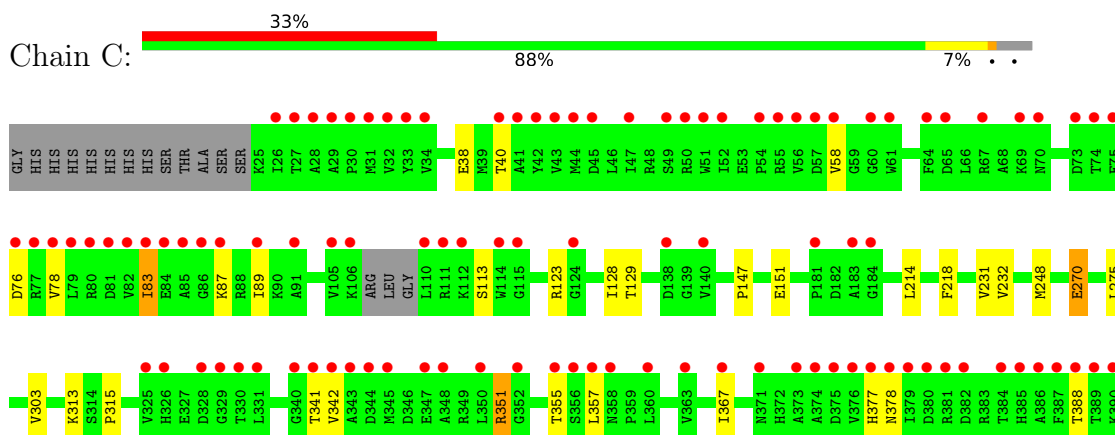
- Molecule 1: Isocitrate dehydrogenase (NAD(+)), mitochondrial

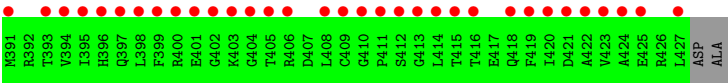


- Molecule 1: Isocitrate dehydrogenase (NAD(+)), mitochondrial

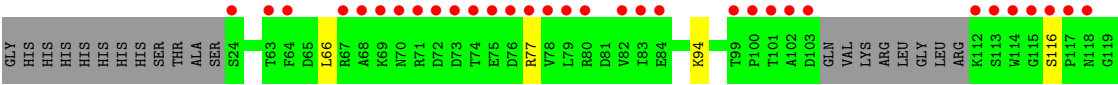
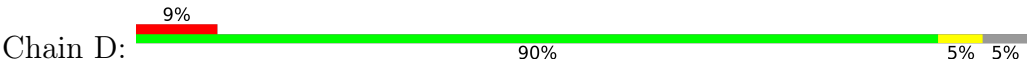


- Molecule 1: Isocitrate dehydrogenase (NAD(+)), mitochondrial





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



4 Data and refinement statistics

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 19.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.9 (19.95-1.80) 94.9 (19.95-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	8825 reflections (4.73%)	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)	0.38 , 36.9	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	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, ICT, MG, GOL, 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	1.06	1/3198 (0.0%)	1.30	2/4333 (0.0%)
1	B	1.04	2/3176 (0.1%)	1.32	4/4310 (0.1%)
1	C	0.98	0/3066	1.32	12/4167 (0.3%)
1	D	1.01	0/3112	1.26	2/4214 (0.0%)
All	All	1.02	3/12552 (0.0%)	1.30	20/17024 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	VAL	C-O	6.08	1.30	1.24
1	B	359	PRO	C-O	-5.69	1.17	1.24
1	B	207	PRO	C-O	-5.01	1.19	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	ILE	N-CA-C	-7.28	106.00	111.90
1	C	78	VAL	N-CA-C	-6.89	102.44	111.05
1	C	128	ILE	N-CA-C	-6.61	105.88	111.56
1	C	377	HIS	CA-C-N	-6.45	114.30	123.20
1	C	377	HIS	C-N-CA	-6.45	114.30	123.20
1	C	270	GLU	CB-CA-C	5.98	119.64	109.72
1	D	328	ASP	CA-CB-CG	5.62	118.22	112.60
1	D	128	ILE	N-CA-C	-5.59	107.37	112.96
1	C	83	ILE	N-CA-CB	5.37	116.83	110.55
1	A	286	GLN	CB-CA-C	-5.26	101.95	110.79
1	A	128	ILE	N-CA-C	-5.23	107.06	111.56
1	B	427	LEU	CA-C-O	5.19	129.62	120.80
1	C	351	ARG	CB-CA-C	5.18	119.33	110.01
1	B	237	VAL	N-CA-C	-5.17	107.71	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ARG	CA-C-N	5.14	125.55	119.94
1	C	123	ARG	C-N-CA	5.14	125.55	119.94
1	C	147	PRO	N-CA-C	5.13	119.26	111.15
1	B	77	ARG	N-CA-C	-5.11	105.35	111.03
1	C	378	ASN	CA-C-N	-5.01	116.43	123.10
1	C	378	ASN	C-N-CA	-5.01	116.43	123.10

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	5	0
1	B	3109	0	2981	9	0
1	C	3000	0	2816	9	0
1	D	3048	0	2949	6	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
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	26	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 (26) 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:94:LYS:HD2	1:D:121:MET:HE1	1.81	0.62
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:C:315:PRO:HG3	1:D:282:MET:HE1	1.92	0.52
1:A:231:VAL:HG22	1:A:248:MET:HE2	1.92	0.50
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:B:33:TYR:C	1:B:33:TYR:CD1	2.97	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:C:231:VAL:HG22	1:C:248:MET:HE2	2.02	0.41
1:A:117:PRO:HB2	1:A:121:MET:HE3	2.02	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

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%)	43 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	402/418 (96%)	393 (98%)	8 (2%)	1 (0%)	43	31
1	C	396/418 (95%)	378 (96%)	16 (4%)	2 (0%)	24	14
1	D	392/418 (94%)	376 (96%)	15 (4%)	1 (0%)	36	25
All	All	1591/1672 (95%)	1537 (97%)	49 (3%)	5 (0%)	36	25

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 ⓘ

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%)	310 (97%)	9 (3%)	38	26
1	B	316/346 (91%)	307 (97%)	9 (3%)	38	26
1	C	292/346 (84%)	282 (97%)	10 (3%)	32	20
1	D	310/346 (90%)	303 (98%)	7 (2%)	44	33
All	All	1237/1384 (89%)	1202 (97%)	35 (3%)	38	26

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	66	LEU
1	A	76	ASP
1	A	249	ARG
1	A	303	VAL
1	A	342	VAL

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Mol	Chain	Res	Type
1	A	345	MET
1	A	357	LEU
1	A	391	MET
1	B	66	LEU
1	B	67	ARG
1	B	76	ASP
1	B	103	ASP
1	B	113	SER
1	B	151	GLU
1	B	221	ARG
1	B	342	VAL
1	B	380	ASP
1	C	76	ASP
1	C	83	ILE
1	C	87	LYS
1	C	89	ILE
1	C	113	SER
1	C	270	GLU
1	C	342	VAL
1	C	351	ARG
1	C	355	THR
1	C	357	LEU
1	D	66	LEU
1	D	77	ARG
1	D	116	SER
1	D	170	LYS
1	D	266	MET
1	D	342	VAL
1	D	380	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	B	310	GLN
1	C	321	ASN
1	D	259	GLN

5.3.3 RNA ⓘ

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 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	$\# Z > 2$
5	IPA	D	502	-	3,3,3	0.31	0	3,3,3	0.10	0
4	FLC	A	502	-	12,12,12	1.07	0	17,17,17	1.01	0
2	ICT	A	500	3	12,12,12	1.30	1 (8%)	13,16,16	1.31	2 (15%)
6	GOL	C	500	-	5,5,5	0.17	0	5,5,5	0.34	0
5	IPA	A	503	-	3,3,3	0.32	0	3,3,3	0.13	0
6	GOL	D	501	-	5,5,5	0.18	0	5,5,5	0.48	0
6	GOL	D	500	-	5,5,5	0.20	0	5,5,5	0.40	0
5	IPA	C	501	-	3,3,3	0.43	0	3,3,3	0.23	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
4	FLC	A	502	-	-	4/16/16/16	-
2	ICT	A	500	3	-	2/16/16/16	-
6	GOL	C	500	-	-	4/4/4/4	-
6	GOL	D	500	-	-	2/4/4/4	-
6	GOL	D	501	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	ICT	O6-C6	-2.05	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	ICT	O7-C2-C3	-2.33	105.38	110.63
2	A	500	ICT	O5-C6-C3	-2.06	118.14	123.01

There are no chirality outliers.

All (16) torsion outliers are listed below:

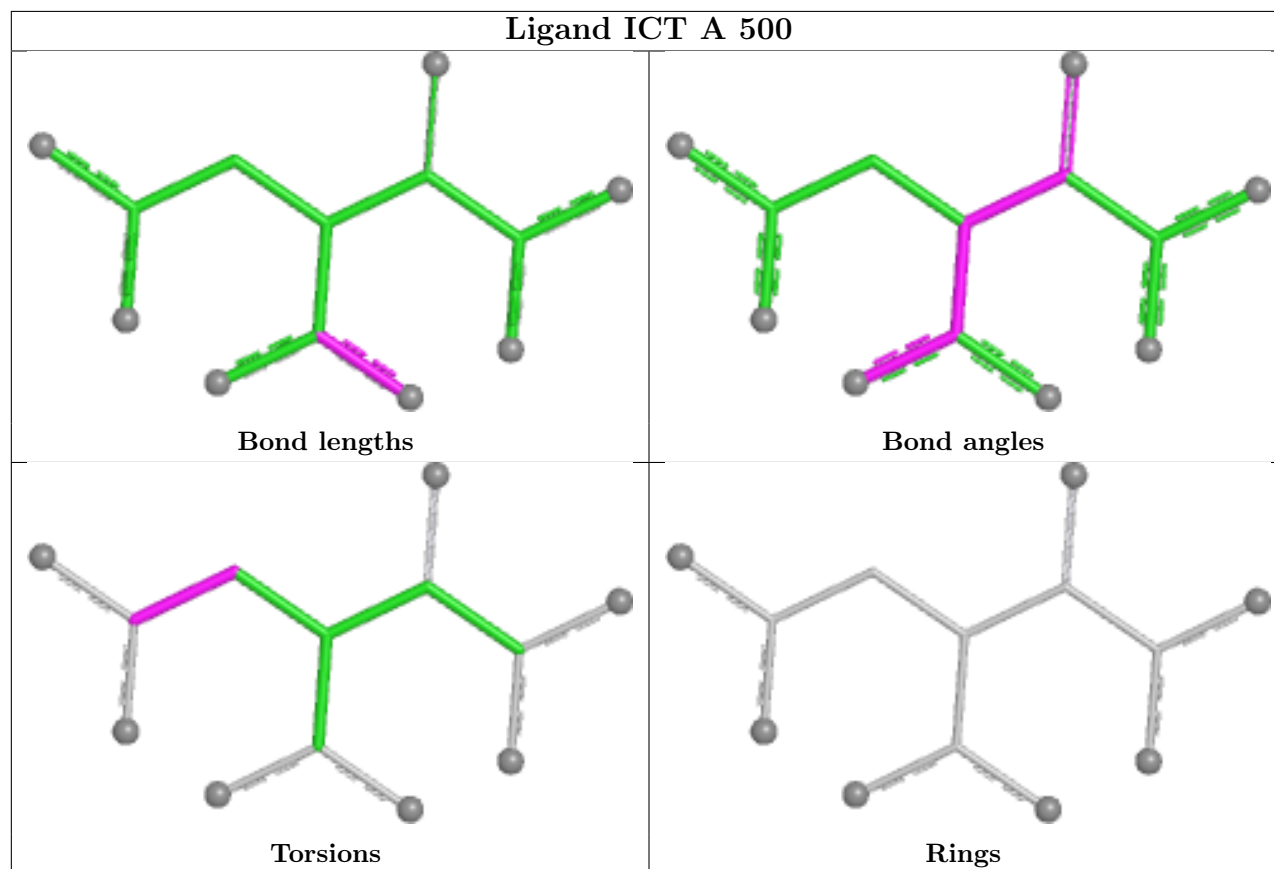
Mol	Chain	Res	Type	Atoms
4	A	502	FLC	CBC-CB-CG-CGC
4	A	502	FLC	OHB-CB-CG-CGC
6	C	500	GOL	C1-C2-C3-O3
6	D	501	GOL	O1-C1-C2-C3
6	D	501	GOL	C1-C2-C3-O3
4	A	502	FLC	CA-CB-CG-CGC
6	C	500	GOL	O1-C1-C2-C3
6	D	500	GOL	C1-C2-C3-O3
6	C	500	GOL	O1-C1-C2-O2
6	C	500	GOL	O2-C2-C3-O3
6	D	501	GOL	O1-C1-C2-O2
6	D	501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

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 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	403/418 (96%)	0.29	17 (4%) 40 40	16, 29, 47, 60	0
1	B	404/418 (96%)	0.26	21 (5%) 33 31	20, 29, 51, 63	0
1	C	400/418 (95%)	1.38	136 (34%) 1 1	17, 37, 64, 88	0
1	D	396/418 (94%)	0.36	37 (9%) 14 12	16, 27, 56, 72	0
All	All	1603/1672 (95%)	0.57	211 (13%) 7 6	16, 29, 57, 88	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	422	ALA	6.9
1	C	355	THR	6.9
1	D	114	TRP	6.6
1	C	110	LEU	6.4
1	C	425	GLU	6.2
1	D	113	SER	6.2
1	D	68	ALA	6.0
1	D	74	THR	5.9
1	C	70	ASN	5.8
1	C	86	GLY	5.8
1	C	413	GLY	5.7
1	D	73	ASP	5.6
1	C	81	ASP	5.5
1	C	378	ASN	5.2
1	D	101	THR	5.1
1	C	401	GLU	5.0
1	B	105	VAL	4.8
1	C	424	ALA	4.8
1	C	52	ILE	4.8
1	A	350	LEU	4.8
1	C	374	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	41	ALA	4.7
1	C	56	VAL	4.7
1	C	111	ARG	4.6
1	C	64	PHE	4.6
1	C	348	ALA	4.6
1	C	343	ALA	4.6
1	C	105	VAL	4.4
1	C	389	THR	4.4
1	D	72	ASP	4.4
1	D	75	GLU	4.4
1	C	411	PRO	4.3
1	D	100	PRO	4.3
1	C	42	TYR	4.3
1	C	394	VAL	4.3
1	D	78	VAL	4.3
1	C	388	THR	4.2
1	C	393	THR	4.2
1	C	390	LYS	4.2
1	C	74	THR	4.1
1	C	78	VAL	4.1
1	C	423	VAL	4.0
1	C	32	VAL	4.0
1	C	83	ILE	4.0
1	C	344	ASP	4.0
1	D	99	THR	4.0
1	A	352	GLY	4.0
1	C	418	GLN	4.0
1	D	76	ASP	3.9
1	C	330	THR	3.9
1	C	347	GLU	3.9
1	C	377	HIS	3.9
1	D	115	GLY	3.8
1	C	387	PHE	3.8
1	C	350	LEU	3.8
1	C	373	ALA	3.8
1	C	47	ILE	3.8
1	C	419	PHE	3.8
1	C	427	LEU	3.7
1	C	375	ASP	3.7
1	C	342	VAL	3.7
1	D	70	ASN	3.7
1	C	51	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	379	ILE	3.6
1	B	180	GLY	3.6
1	C	404	GLY	3.6
1	C	380	ASP	3.6
1	C	402	GLY	3.5
1	C	31	MET	3.5
1	B	120	ALA	3.5
1	C	414	LEU	3.5
1	B	114	TRP	3.5
1	C	386	ALA	3.5
1	C	328	ASP	3.5
1	C	26	ILE	3.4
1	C	395	ILE	3.4
1	C	326	HIS	3.4
1	D	83	ILE	3.4
1	C	65	ASP	3.3
1	C	409	CYS	3.3
1	C	124	GLY	3.3
1	C	410	GLY	3.3
1	C	40	THR	3.3
1	C	341	THR	3.3
1	C	181	PRO	3.3
1	D	103	ASP	3.3
1	C	112	LYS	3.2
1	C	352	GLY	3.2
1	C	367	ILE	3.2
1	C	420	ILE	3.2
1	D	67	ARG	3.2
1	C	75	GLU	3.2
1	B	269	GLY	3.2
1	C	87	LYS	3.2
1	C	412	SER	3.2
1	C	396	HIS	3.2
1	C	58	VAL	3.2
1	C	325	VAL	3.2
1	C	28	ALA	3.1
1	C	397	GLN	3.1
1	C	398	LEU	3.1
1	D	24	SER	3.1
1	D	80	ARG	3.1
1	C	60	GLY	3.1
1	B	110	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	57	ASP	3.1
1	C	27	THR	3.1
1	B	119	GLY	3.1
1	C	371	ASN	3.0
1	C	106	LYS	3.0
1	C	357	LEU	3.0
1	D	69	LYS	3.0
1	C	385	HIS	3.0
1	C	381	ARG	2.9
1	C	30	PRO	2.9
1	C	400	ARG	2.9
1	C	415	THR	2.9
1	C	54	PRO	2.9
1	A	343	ALA	2.8
1	B	103	ASP	2.8
1	D	116	SER	2.8
1	C	358	ASN	2.8
1	D	117	PRO	2.8
1	D	102	ALA	2.8
1	D	77	ARG	2.8
1	B	183	ALA	2.8
1	C	399	PHE	2.8
1	A	353	GLU	2.8
1	C	384	THR	2.8
1	D	79	LEU	2.8
1	C	34	VAL	2.8
1	D	120	ALA	2.7
1	C	331	LEU	2.7
1	B	111	ARG	2.7
1	D	64	PHE	2.7
1	C	356	SER	2.7
1	C	91	ALA	2.7
1	C	184	GLY	2.7
1	B	78	VAL	2.7
1	B	102	ALA	2.6
1	C	345	MET	2.6
1	A	25	LYS	2.6
1	C	363	VAL	2.6
1	C	77	ARG	2.6
1	C	408	LEU	2.6
1	C	421	ASP	2.6
1	B	74	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	114	TRP	2.6
1	C	329	GLY	2.6
1	C	85	ALA	2.6
1	B	106	LYS	2.5
1	D	118	ASN	2.5
1	C	76	ASP	2.5
1	C	138	ASP	2.5
1	C	89	ILE	2.5
1	C	382	ASP	2.5
1	C	33	TYR	2.5
1	C	79	LEU	2.5
1	A	348	ALA	2.5
1	C	405	THR	2.4
1	D	344	ASP	2.4
1	B	181	PRO	2.4
1	D	261	VAL	2.4
1	C	80	ARG	2.4
1	C	416	THR	2.3
1	D	262	ALA	2.3
1	D	124	GLY	2.3
1	C	376	VAL	2.3
1	C	84	GLU	2.3
1	C	29	ALA	2.3
1	D	82	VAL	2.3
1	B	262	ALA	2.3
1	C	406	ARG	2.3
1	A	425	GLU	2.3
1	C	44	MET	2.3
1	C	391	MET	2.3
1	D	71	ARG	2.2
1	B	72	ASP	2.2
1	C	82	VAL	2.2
1	C	403	LYS	2.2
1	C	55	ARG	2.2
1	C	360	LEU	2.2
1	D	84	GLU	2.2
1	A	54	PRO	2.2
1	C	49	SER	2.2
1	C	45	ASP	2.2
1	A	42	TYR	2.2
1	A	378	ASN	2.2
1	D	112	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	63	THR	2.2
1	A	49	SER	2.2
1	C	340	GLY	2.2
1	A	420	ILE	2.1
1	C	140	VAL	2.1
1	C	50	ARG	2.1
1	C	67	ARG	2.1
1	A	217	PHE	2.1
1	B	77	ARG	2.1
1	C	115	GLY	2.1
1	B	24	SER	2.1
1	A	186	THR	2.1
1	A	355	THR	2.1
1	B	266	MET	2.1
1	C	43	VAL	2.1
1	C	73	ASP	2.1
1	C	69	LYS	2.0
1	C	61	TRP	2.0
1	B	258	ALA	2.0
1	C	183	ALA	2.0
1	A	346	ASP	2.0
1	A	347	GLU	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	GOL	C	500	6/6	0.76	0.17	45,54,54,55	0

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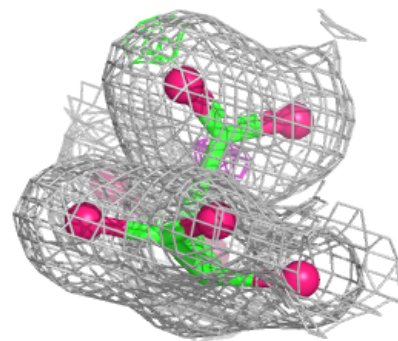
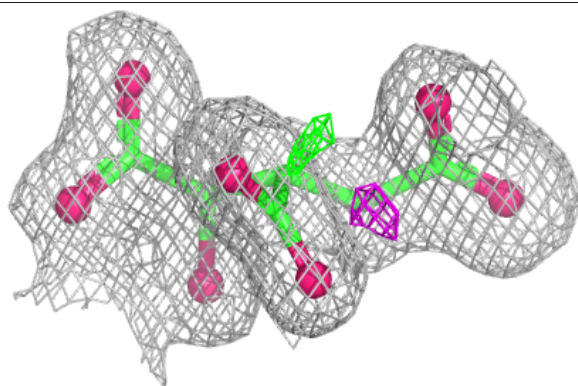
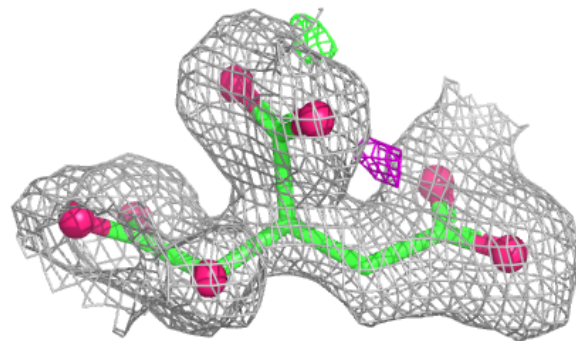
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	IPA	D	502	4/4	0.82	0.18	38,40,42,44	0
4	FLC	A	502	13/13	0.83	0.12	32,41,64,74	0
5	IPA	C	501	4/4	0.84	0.16	31,37,37,41	0
6	GOL	D	500	6/6	0.85	0.10	38,42,45,48	0
6	GOL	D	501	6/6	0.86	0.13	28,36,36,50	0
5	IPA	A	503	4/4	0.89	0.15	34,38,38,41	0
2	ICT	A	500	13/13	0.94	0.07	23,27,33,33	0
3	MG	A	501	1/1	0.99	0.04	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.

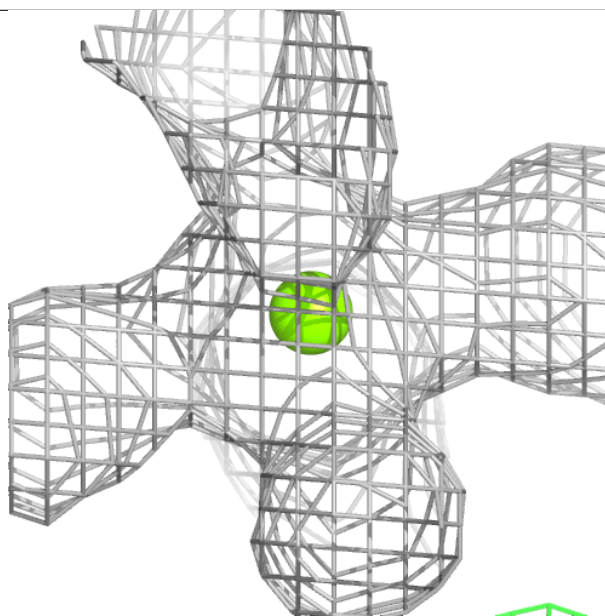
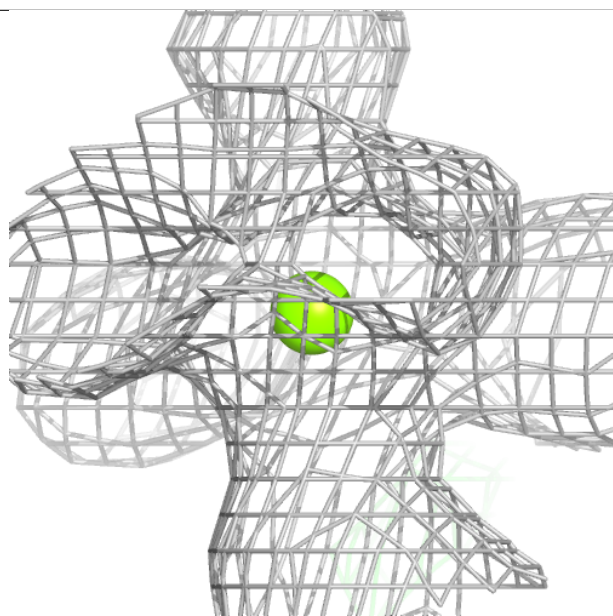
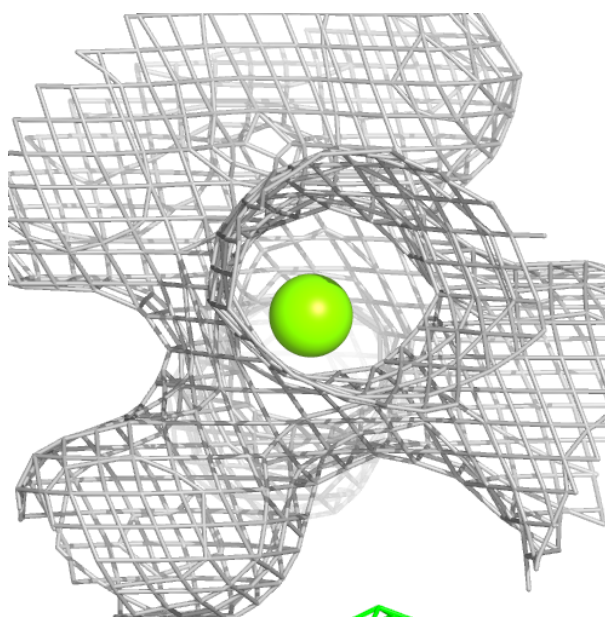
Electron density around ICT A 500:

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.