



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:08 PM UTC

PDB ID : 7TN6 / pdb_00007tn6
Title : Crystal structure of Zea mays Inositol-tetrakisphosphate Kinase 1 mutant (ZmITPK1-H192A)
Authors : Zong, G.; Wang, H.; Shears, S.B.
Deposited on : 2022-01-20
Resolution : 2.85 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

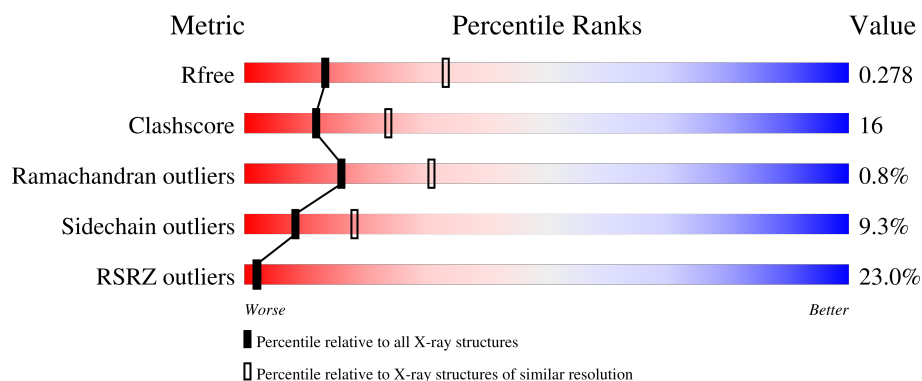
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2086 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 Inositol-tetrakisphosphate 1-kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2069	1345	364	353	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	ALA	HIS	engineered mutation	UNP Q84Y01

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

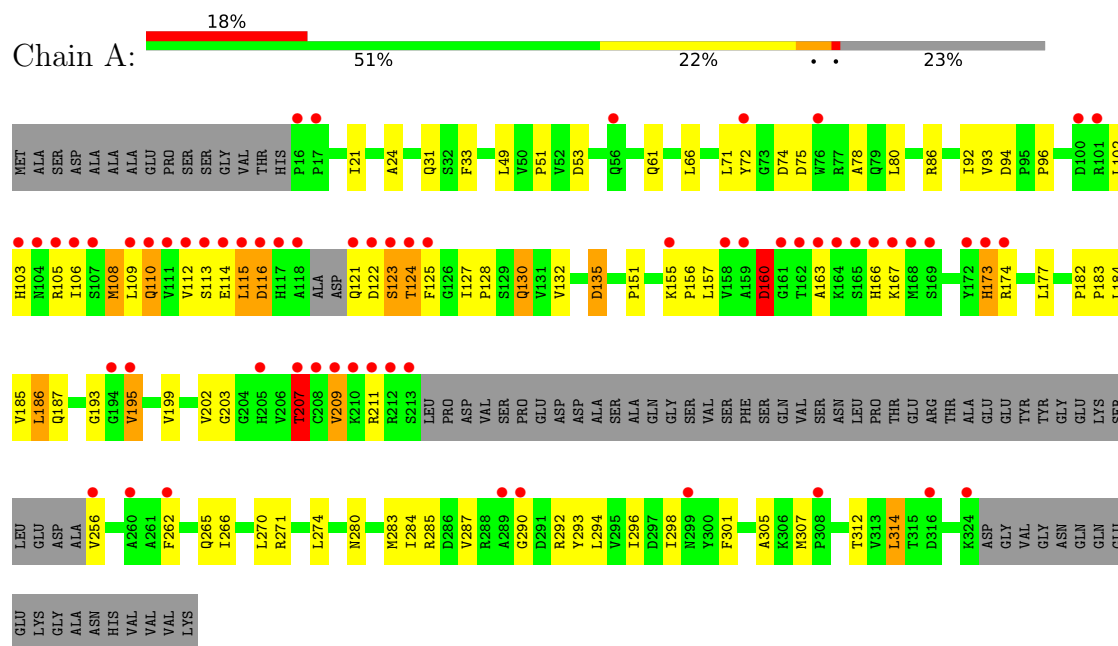
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		

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: Inositol-tetrakisphosphate 1-kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.16Å 98.16Å 202.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.74 – 2.85 47.74 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.74-2.85) 97.6 (47.74-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.48 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.224 , 0.271 (Not available) , 0.278	Depositor DCC
R_{free} test set	700 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2086	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: 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	1.15	3/2124 (0.1%)	1.48	12/2887 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	GLN	C-O	7.00	1.32	1.24
1	A	301	PHE	C-O	-5.67	1.21	1.23
1	A	51	PRO	C-O	-5.07	1.18	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	THR	CB-CA-C	7.00	123.21	109.35
1	A	74	ASP	N-CA-C	-6.26	104.55	111.82
1	A	114	GLU	N-CA-C	5.98	118.57	111.33
1	A	151	PRO	CA-C-N	5.67	130.99	122.99
1	A	151	PRO	C-N-CA	5.67	130.99	122.99
1	A	160	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	31	GLN	N-CA-C	-5.22	105.48	111.07
1	A	312	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	305	ALA	N-CA-C	-5.14	106.85	113.01
1	A	265	GLN	CA-C-N	5.02	126.99	120.56
1	A	265	GLN	C-N-CA	5.02	126.99	120.56
1	A	114	GLU	CA-C-O	-5.02	115.21	120.63

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	2069	0	2099	66	0
2	A	1	0	0	0	0
3	A	16	0	0	2	0
All	All	2086	0	2099	66	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 16.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:CG2	1:A:298:ILE:HD11	1.56	1.33
1:A:112:VAL:CG2	1:A:298:ILE:CD1	2.34	1.04
1:A:112:VAL:HG22	1:A:298:ILE:HD11	1.46	0.97
1:A:112:VAL:HG23	1:A:298:ILE:CD1	2.00	0.91
1:A:112:VAL:HG21	1:A:298:ILE:HD11	1.54	0.89
1:A:173:HIS:CE1	3:A:714:HOH:O	2.30	0.83
1:A:115:LEU:O	1:A:125:PHE:HZ	1.65	0.77
1:A:193:GLY:HA3	1:A:287:VAL:HG11	1.73	0.70
1:A:209:VAL:HG23	3:A:706:HOH:O	1.93	0.68
1:A:262:PHE:CE2	1:A:266:ILE:HD11	2.31	0.65
1:A:199:VAL:O	1:A:280:ASN:HB2	1.97	0.64
1:A:105:ARG:NH2	1:A:296:ILE:O	2.32	0.62
1:A:112:VAL:HG23	1:A:298:ILE:HD12	1.78	0.62
1:A:207:THR:HG21	1:A:307:MET:CE	2.29	0.61
1:A:128:PRO:HG2	1:A:187:GLN:HE22	1.66	0.60
1:A:266:ILE:HD13	1:A:283:MET:HE1	1.85	0.58
1:A:115:LEU:O	1:A:125:PHE:CZ	2.53	0.58
1:A:24:ALA:HB1	1:A:71:LEU:CD1	2.34	0.58
1:A:86:ARG:HA	1:A:86:ARG:HE	1.70	0.57
1:A:182:PRO:HA	1:A:183:PRO:C	2.30	0.57
1:A:135:ASP:N	1:A:135:ASP:OD1	2.38	0.56
1:A:80:LEU:HD13	1:A:96:PRO:HG3	1.88	0.55
1:A:283:MET:HA	1:A:294:LEU:O	2.08	0.54
1:A:266:ILE:CD1	1:A:283:MET:HE1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HD11	1:A:132:VAL:HG22	1.90	0.53
1:A:157:LEU:HD13	1:A:185:VAL:CG2	2.39	0.53
1:A:102:LEU:HD21	1:A:274:LEU:HD22	1.90	0.52
1:A:24:ALA:HB1	1:A:71:LEU:HD11	1.91	0.52
1:A:112:VAL:HG22	1:A:270:LEU:HD21	1.91	0.52
1:A:125:PHE:HA	1:A:293:TYR:O	2.10	0.52
1:A:124:THR:HB	1:A:292:ARG:HG3	1.93	0.51
1:A:21:ILE:HB	1:A:49:LEU:HD23	1.93	0.51
1:A:21:ILE:HG23	1:A:66:LEU:HD23	1.92	0.51
1:A:105:ARG:HG2	1:A:108:MET:CE	2.40	0.50
1:A:112:VAL:HG22	1:A:270:LEU:CD2	2.42	0.50
1:A:102:LEU:HD21	1:A:274:LEU:CD2	2.41	0.49
1:A:116:ASP:HA	1:A:125:PHE:CZ	2.47	0.49
1:A:195:VAL:O	1:A:284:ILE:HG22	2.12	0.49
1:A:113:SER:HA	1:A:127:ILE:HD11	1.94	0.49
1:A:193:GLY:CA	1:A:287:VAL:HG11	2.42	0.49
1:A:105:ARG:HG3	1:A:155:LYS:HD3	1.95	0.48
1:A:109:LEU:HB3	1:A:127:ILE:HG21	1.96	0.48
1:A:53:ASP:O	1:A:61:GLN:NE2	2.46	0.48
1:A:53:ASP:HB3	1:A:61:GLN:NE2	2.30	0.47
1:A:280:ASN:OD1	1:A:280:ASN:C	2.57	0.46
1:A:72:TYR:CD1	1:A:103:HIS:HE1	2.34	0.46
1:A:109:LEU:CD1	1:A:130:GLN:OE1	2.63	0.46
1:A:80:LEU:HD22	1:A:92:ILE:HD13	1.98	0.46
1:A:105:ARG:HG2	1:A:108:MET:HE2	1.97	0.46
1:A:285:ARG:HH11	1:A:290:GLY:HA2	1.81	0.46
1:A:121:GLN:HE21	1:A:123:SER:H	1.64	0.45
1:A:72:TYR:CD2	1:A:160:ASP:HB2	2.52	0.45
1:A:93:VAL:HA	1:A:94:ASP:HA	1.63	0.45
1:A:177:LEU:HD11	1:A:186:LEU:HD21	1.99	0.45
1:A:285:ARG:NH1	1:A:290:GLY:HA2	2.33	0.44
1:A:33:PHE:HZ	1:A:314:LEU:HD22	1.83	0.44
1:A:75:ASP:O	1:A:78:ALA:HB3	2.18	0.44
1:A:112:VAL:HG22	1:A:298:ILE:CD1	2.29	0.43
1:A:128:PRO:HG2	1:A:187:GLN:NE2	2.33	0.43
1:A:72:TYR:CD1	1:A:103:HIS:CE1	3.06	0.43
1:A:256:VAL:O	1:A:256:VAL:HG13	2.19	0.43
1:A:121:GLN:OE1	1:A:262:PHE:HD1	2.01	0.43
1:A:155:LYS:HG2	1:A:156:PRO:HD2	2.02	0.41
1:A:202:VAL:O	1:A:203:GLY:C	2.62	0.41
1:A:284:ILE:O	1:A:293:TYR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ALA:HB3	1:A:166:HIS:CD2	2.57	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	259/342 (76%)	243 (94%)	14 (5%)	2 (1%)	16 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	ASP
1	A	211	ARG

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	216/277 (78%)	196 (91%)	20 (9%)	8 18

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	MET

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Mol	Chain	Res	Type
1	A	110	GLN
1	A	115	LEU
1	A	116	ASP
1	A	122	ASP
1	A	123	SER
1	A	124	THR
1	A	130	GLN
1	A	135	ASP
1	A	160	ASP
1	A	167	LYS
1	A	173	HIS
1	A	174	ARG
1	A	184	LEU
1	A	186	LEU
1	A	195	VAL
1	A	207	THR
1	A	209	VAL
1	A	271	ARG
1	A	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	104	ASN
1	A	110	GLN
1	A	117	HIS
1	A	130	GLN
1	A	173	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	265/342 (77%)	1.05	61 (23%) 2 2	22, 50, 121, 151	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	ALA	7.6
1	A	155	LYS	7.1
1	A	161	GLY	6.8
1	A	167	LYS	5.9
1	A	111	VAL	5.9
1	A	112	VAL	5.5
1	A	166	HIS	5.5
1	A	324	LYS	5.3
1	A	162	THR	5.3
1	A	195	VAL	5.0
1	A	123	SER	5.0
1	A	117	HIS	4.9
1	A	121	GLN	4.6
1	A	210	LYS	4.5
1	A	115	LEU	4.3
1	A	16	PRO	4.2
1	A	72	TYR	4.2
1	A	207	THR	4.2
1	A	163	ALA	4.2
1	A	213	SER	4.2
1	A	159	ALA	4.0
1	A	164	LYS	4.0
1	A	116	ASP	3.9
1	A	290	GLY	3.7
1	A	208	CYS	3.6
1	A	316	ASP	3.5
1	A	262	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	168	MET	3.4
1	A	124	THR	3.4
1	A	205	HIS	3.4
1	A	122	ASP	3.2
1	A	194	GLY	3.2
1	A	211	ARG	3.2
1	A	105	ARG	3.1
1	A	209	VAL	3.1
1	A	101	ARG	3.0
1	A	308	PRO	3.0
1	A	256	VAL	2.9
1	A	212	ARG	2.9
1	A	289	ALA	2.9
1	A	103	HIS	2.8
1	A	106	ILE	2.8
1	A	158	VAL	2.8
1	A	125	PHE	2.6
1	A	56	GLN	2.6
1	A	172	TYR	2.6
1	A	109	LEU	2.6
1	A	260	ALA	2.6
1	A	174	ARG	2.5
1	A	299	ASN	2.3
1	A	100	ASP	2.3
1	A	173	HIS	2.3
1	A	110	GLN	2.2
1	A	107	SER	2.2
1	A	113	SER	2.2
1	A	17	PRO	2.2
1	A	114	GLU	2.2
1	A	104	ASN	2.1
1	A	165	SER	2.1
1	A	169	SER	2.0
1	A	76	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

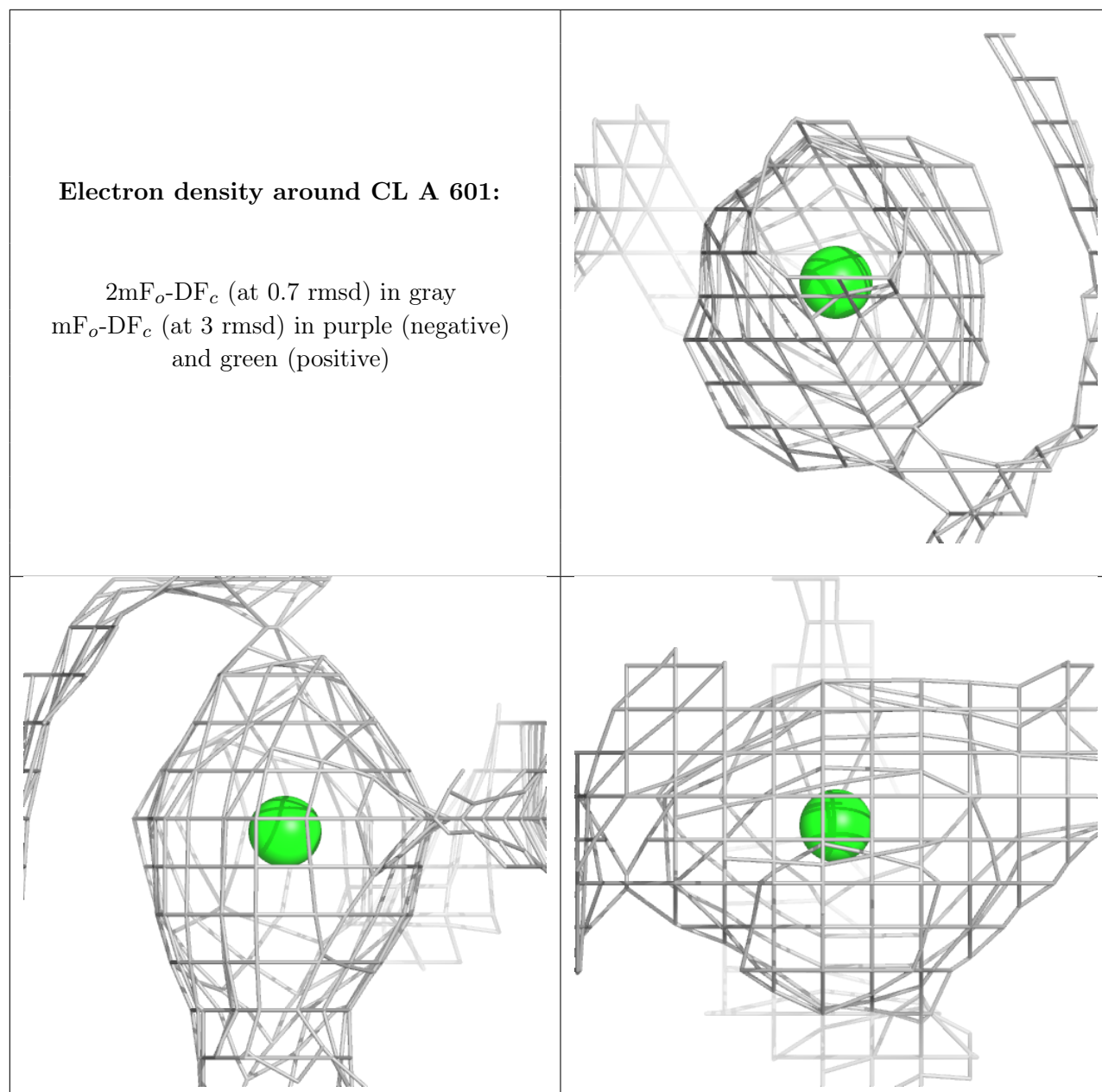
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	CL	A	601	1/1	0.99	0.09	28,28,28,28	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.