



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:01 PM UTC

PDB ID : 6K4K / pdb_00006k4k
Title : Crystal structure of SidJ-CaM binary complex at 2.71 Å
Authors : Ouyang, S.Y.
Deposited on : 2019-05-24
Resolution : 2.71 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 ⓘ 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

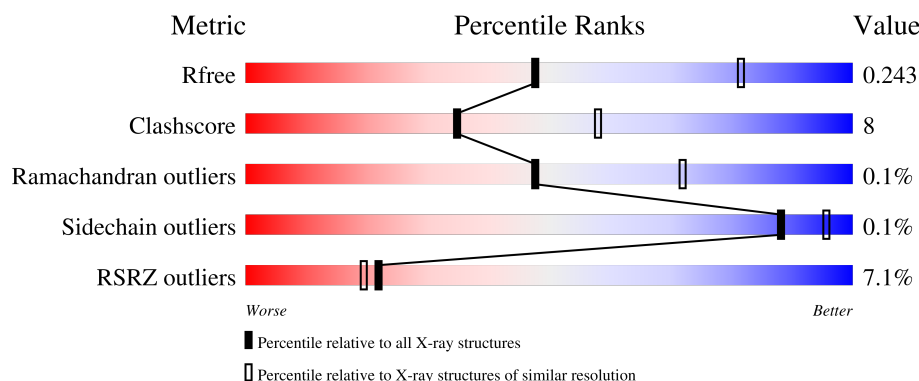
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	873	3% 72% 12% 16%
1	B	873	2% 72% 12% 16%
2	C	149	25% 54% 26% 19%
2	D	149	23% 42% 20% 36%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13093 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 SidJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	734	Total	C	N	O	S	0	0	0
			5725	3674	958	1079	14			
1	B	737	Total	C	N	O	S	0	0	0
			5785	3711	968	1091	15			

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	120	Total	C	N	O	S	0	0	0
			882	538	142	197	5			
2	D	95	Total	C	N	O	S	0	0	0
			697	426	110	157	4			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

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.

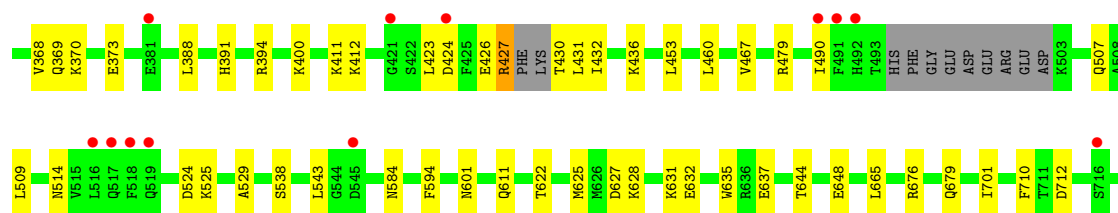
[illegible]

Chain B:

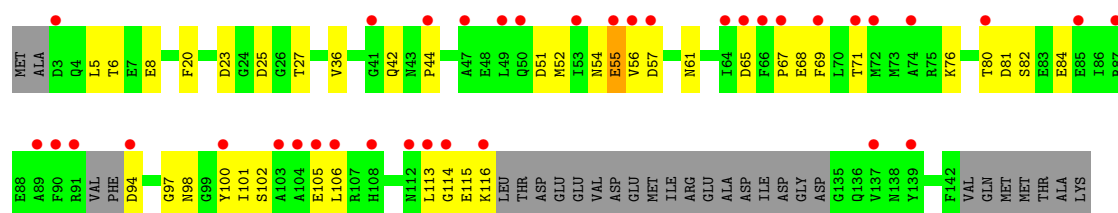
72% 12% 16%

2%

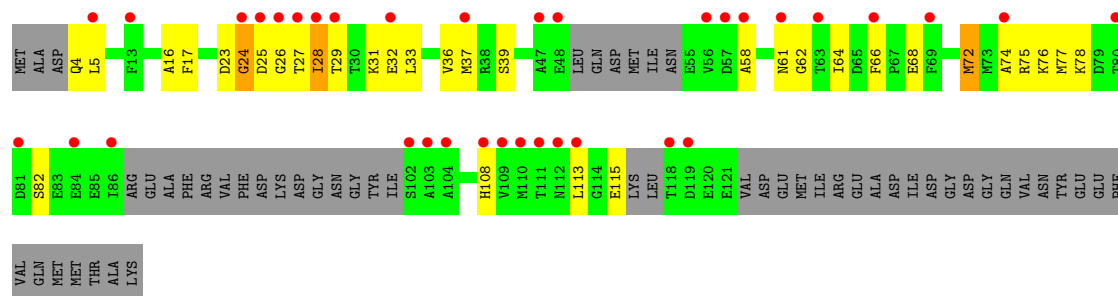
Residue	Category
VAL	Green
LYS	Green
PRO	Green
GLU	Green
THR	Green
ILE	Green
ALA	Green
PRO	Green
ASP	Green
GLN	Green
LYS	Green
LYS	Green
HIS	Green
GLN	Green
ILE	Green
LYS	Green
THR	Green
GLU	Green
THR	Green
THR	Green
LYS	Green
GLN	Green
LYS	Green
GLY	Green
PRO	Green
LYS	Green
VAL	Green
THR	Green
LEU	Green
MET	Green
ASP	Green
GLY	Green
HIS	Green
V99	Green
Y103	Yellow
R107	Yellow
D114	Yellow
L117	Yellow
P118	Yellow
S128	Red
I134	Yellow
E137	Yellow
R140	Yellow
N141	Yellow
Q145	Yellow



● Molecule 2: Calmodulin-1



● Molecule 2: Calmodulin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.95Å 159.53Å 135.61Å 90.00° 101.89° 90.00°	Depositor
Resolution (Å)	55.87 – 2.71 55.87 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.9 (55.87-2.71) 96.9 (55.87-2.71)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.205 , 0.243 0.207 , 0.243	Depositor DCC
R_{free} test set	1995 reflections (2.92%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13093	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: CA

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	0.29	2/5855 (0.0%)	0.52	1/7961 (0.0%)
1	B	0.29	2/5917 (0.0%)	0.49	2/8036 (0.0%)
2	C	0.31	0/888	0.67	2/1197 (0.2%)
2	D	0.30	0/701	0.80	1/941 (0.1%)
All	All	0.29	4/13361 (0.0%)	0.54	6/18135 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	D	0	3
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	134	ILE	CA-C	6.71	1.58	1.53
1	A	719	GLY	C-O	6.22	1.27	1.24
1	A	134	ILE	CA-C	-5.54	1.49	1.53
1	B	719	GLY	C-O	5.20	1.27	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	64	ILE	N-CA-C	-7.21	105.75	112.96
1	B	134	ILE	CA-C-O	-5.34	116.13	119.12
1	B	134	ILE	O-C-N	5.33	125.33	121.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	811	GLU	N-CA-CB	-5.04	102.69	110.20
2	C	55	GLU	CA-C-N	-5.02	112.93	121.97

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	435	SER	Peptide
2	D	24	GLY	Peptide
2	D	28	ILE	Peptide
2	D	72	MET	Peptide

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	5725	0	5510	70	0
1	B	5785	0	5593	78	0
2	C	882	0	775	30	0
2	D	697	0	620	24	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
All	All	13093	0	12498	192	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 8.

The worst 5 of 192 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)
2:D:78:LYS:HE3	2:D:82:SER:OG	1.61	0.98
1:A:430:THR:HG23	1:A:431:LEU:HD12	1.64	0.78
2:D:28:ILE:O	2:D:29:THR:HG23	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:ARG:H	2:D:24:GLY:H	1.33	0.74
1:A:507:GLN:HE22	1:A:514:ASN:HD21	1.34	0.74

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	728/873 (83%)	696 (96%)	32 (4%)	0	100	100
1	B	731/873 (84%)	694 (95%)	37 (5%)	0	100	100
2	C	114/149 (76%)	98 (86%)	16 (14%)	0	100	100
2	D	87/149 (58%)	60 (69%)	25 (29%)	2 (2%)	5	12
All	All	1660/2044 (81%)	1548 (93%)	110 (7%)	2 (0%)	48	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	26	GLY
2	D	108	HIS

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	604/794 (76%)	604 (100%)	0	100	100
1	B	616/794 (78%)	615 (100%)	1 (0%)	87	95
2	C	87/127 (68%)	87 (100%)	0	100	100
2	D	71/127 (56%)	70 (99%)	1 (1%)	59	80
All	All	1378/1842 (75%)	1376 (100%)	2 (0%)	88	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	427	ARG
2	D	115	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	507	GLN
1	B	601	ASN
1	B	584	ASN
1	B	679	GLN
1	A	601	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	734/873 (84%)	0.24	28 (3%)	44 40	35, 62, 100, 131	0
1	B	737/873 (84%)	0.12	20 (2%)	56 53	37, 60, 101, 140	0
2	C	120/149 (80%)	1.49	37 (30%)	1 1	45, 98, 143, 172	0
2	D	95/149 (63%)	1.70	35 (36%)	1 1	51, 101, 141, 185	0
All	All	1686/2044 (82%)	0.36	120 (7%)	22 19	35, 63, 117, 185	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	57	ASP	10.7
2	D	113	LEU	6.6
2	C	105	GLU	6.5
2	D	26	GLY	5.2
2	D	63	THR	4.8

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](#)

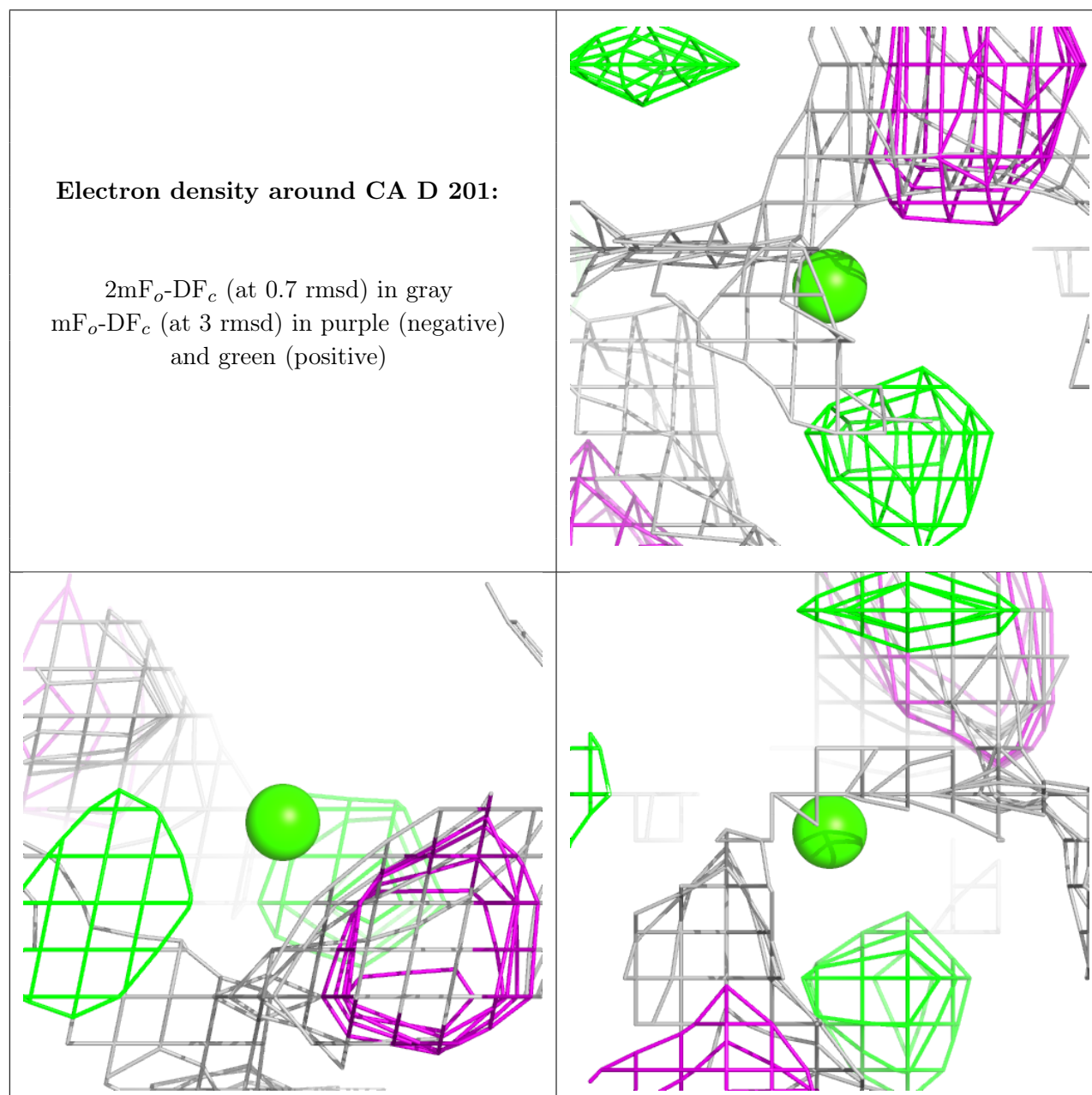
There are no oligosaccharides in this entry.

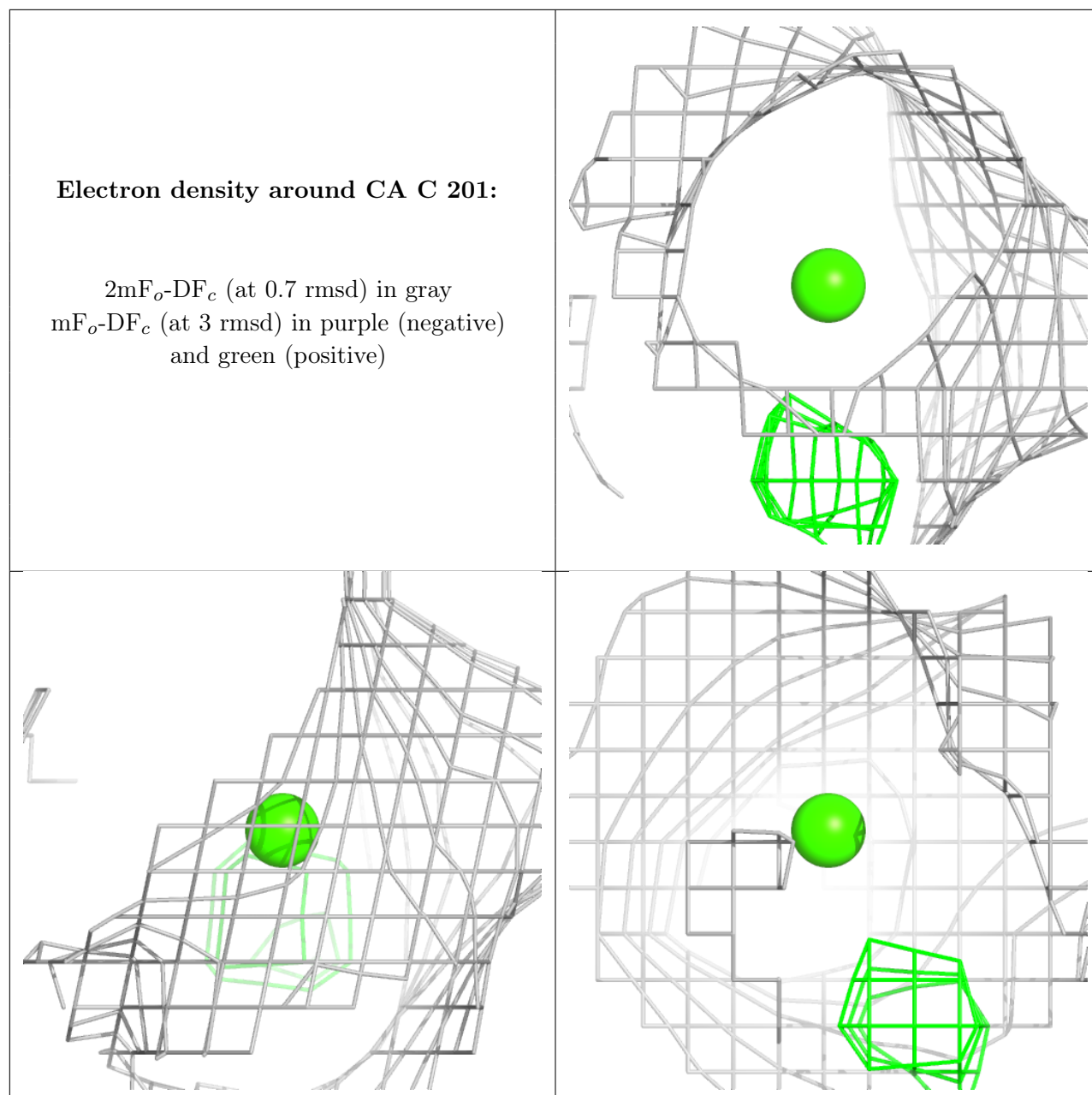
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	CA	D	201	1/1	0.74	0.12	157,157,157,157	0
3	CA	C	201	1/1	0.90	0.08	99,99,99,99	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.