



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 07:47 PM UTC

PDB ID : 8T7C / pdb_00008t7c
Title : Crystal structure of human phospholipase C gamma 2
Authors : Chen, Y.; Choi, H.; Zhuang, N.; Hu, L.; Qian, D.; Wang, J.
Deposited on : 2023-06-20
Resolution : 2.55 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
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

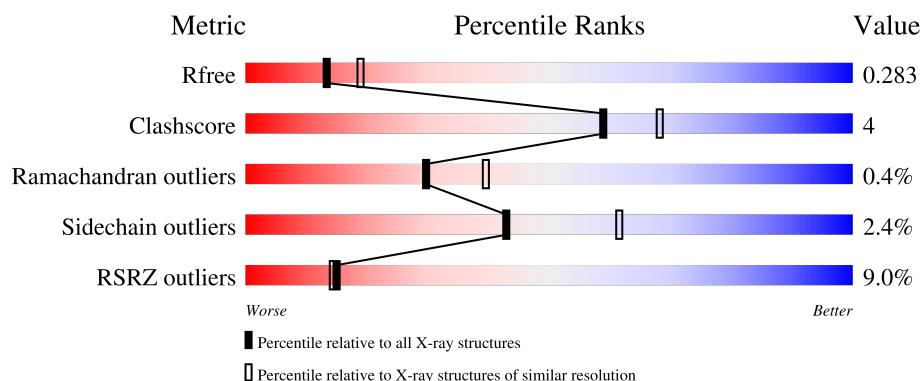
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	1166	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8400 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 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1001	Total	C	N	O	S	0	1	0
			8205	5230	1403	1530	42			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	SER	-	expression tag	UNP P16885
A	12	ILE	-	expression tag	UNP P16885
A	13	ALA	-	expression tag	UNP P16885
A	222	GLY	-	linker	UNP P16885
A	223	SER	-	linker	UNP P16885
A	224	GLY	-	linker	UNP P16885

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	190	Total	O	0	0
			190	190		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.34Å 97.14Å 180.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.62 – 2.55 48.62 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.62-2.55) 99.7 (48.62-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.227 , 0.282 0.229 , 0.283	Depositor DCC
R_{free} test set	2243 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.4	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	0.93	EDS
Total number of atoms	8400	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: EDO, 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	0.98	0/8400	1.36	2/11342 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	221	PHE	CA-C-N	5.28	126.19	120.44
1	A	221	PHE	C-N-CA	5.28	126.19	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	8205	0	8092	72	0
2	A	1	0	0	0	0
3	A	4	0	6	0	0
4	A	190	0	0	1	0
All	All	8400	0	8098	72	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 4.

All (72) 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:1113:TRP:O	1:A:1116:THR:HG22	1.88	0.74
1:A:682:ILE:HG23	1:A:693:CYS:HB2	1.74	0.70
1:A:309:VAL:HG23	4:A:1448:HOH:O	1.92	0.68
1:A:150:ILE:HG21	1:A:161:ILE:HD11	1.80	0.64
1:A:158:ARG:NH1	1:A:165:GLU:OE1	2.32	0.62
1:A:241:VAL:HG13	1:A:285:LEU:HB2	1.82	0.61
1:A:661:MET:HE3	1:A:690:VAL:HG23	1.82	0.61
1:A:1039:GLN:O	1:A:1044:ARG:NH2	2.32	0.61
1:A:1004:LEU:HD12	1:A:1092:ALA:HB3	1.83	0.61
1:A:186:LYS:C	1:A:190:ILE:HD12	2.26	0.61
1:A:412:GLU:OE2	1:A:415:ARG:NH1	2.36	0.59
1:A:407:GLU:OE2	1:A:417:MET:HE1	2.04	0.58
1:A:482:TYR:HB2	1:A:889:ALA:HB3	1.85	0.58
1:A:190:ILE:HG23	1:A:204:LEU:HD23	1.85	0.58
1:A:394:PHE:HA	1:A:397:SER:O	2.04	0.57
1:A:1088:GLU:HB3	1:A:1098:LYS:HB3	1.86	0.56
1:A:303:ASP:HA	1:A:1159:LYS:HD2	1.88	0.55
1:A:702:PHE:CE2	1:A:713:LEU:HD11	2.41	0.55
1:A:693:CYS:SG	1:A:1141:MET:HE2	2.47	0.55
1:A:77:LYS:HA	1:A:82:PHE:CD2	2.44	0.53
1:A:454:LYS:HD2	1:A:955:ILE:HD13	1.91	0.52
1:A:336:LEU:HD11	1:A:992:VAL:CG1	2.41	0.51
1:A:755:VAL:HG13	1:A:758:MET:HE2	1.93	0.50
1:A:1101:THR:HA	1:A:1117:GLN:HE22	1.76	0.50
1:A:802:GLU:HB3	1:A:803:PRO:HD2	1.94	0.50
1:A:336:LEU:HD11	1:A:992:VAL:HG11	1.94	0.50
1:A:102:THR:HG22	1:A:1169:ASN:ND2	2.28	0.49
1:A:758:MET:HE3	1:A:759:TYR:CZ	2.48	0.48
1:A:650:SER:O	1:A:650:SER:OG	2.26	0.48
1:A:363:GLY:HA3	1:A:367:LYS:O	2.14	0.48
1:A:417:MET:HE2	1:A:930:LEU:HD22	1.97	0.47
1:A:1061:MET:HE3	1:A:1186:MET:CG	2.45	0.46
1:A:186:LYS:O	1:A:189:GLU:N	2.49	0.46
1:A:170:LEU:N	1:A:171:PRO:HD2	2.30	0.46
1:A:1130:ALA:HB3	1:A:1155:ILE:HD12	1.98	0.45
1:A:1064:THR:HG22	1:A:1121:THR:HG23	1.98	0.45
1:A:1110:SER:N	1:A:1111:PRO:HD3	2.32	0.45
1:A:154:ASP:OD1	1:A:154:ASP:C	2.60	0.45
1:A:706:THR:HG21	1:A:1106:ASP:OD2	2.17	0.45
1:A:950[A]:PRO:HB3	1:A:977:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:LYS:HE3	1:A:677:SER:O	2.18	0.44
1:A:950[B]:PRO:HB3	1:A:977:TYR:CD2	2.52	0.44
1:A:694:ARG:HE	1:A:696:ASN:HD21	1.66	0.44
1:A:693:CYS:SG	1:A:1142:PHE:CZ	3.11	0.44
1:A:1160:SER:N	1:A:1186:MET:HE1	2.33	0.44
1:A:145:TRP:O	1:A:149:GLN:HG2	2.18	0.43
1:A:330:TYR:OH	1:A:359:ASP:OD2	2.25	0.43
1:A:668:ALA:HA	1:A:733:TYR:HB2	2.01	0.43
1:A:736:THR:HB	1:A:737:PRO:HD2	2.01	0.43
1:A:208:LYS:O	1:A:212:GLU:HG2	2.18	0.43
1:A:187:PHE:HB3	1:A:192:ALA:HB2	2.00	0.42
1:A:150:ILE:CG2	1:A:161:ILE:HD11	2.49	0.42
1:A:241:VAL:CG1	1:A:285:LEU:HB2	2.49	0.42
1:A:984:ARG:HA	1:A:1009:MET:O	2.20	0.42
1:A:186:LYS:O	1:A:190:ILE:HD12	2.20	0.42
1:A:769:MET:HG2	1:A:798:ASN:OD1	2.20	0.42
1:A:187:PHE:C	1:A:192:ALA:HB2	2.44	0.41
1:A:214:GLN:HA	1:A:1112:ILE:HD11	2.02	0.41
1:A:970:LYS:N	1:A:971:PRO:CD	2.83	0.41
1:A:1102:THR:OG1	1:A:1116:THR:HG21	2.20	0.41
1:A:163:LEU:O	1:A:163:LEU:HD23	2.21	0.41
1:A:399:PHE:HB3	1:A:400:PRO:HD2	2.03	0.41
1:A:151:TYR:CZ	1:A:157:ARG:HG3	2.56	0.41
1:A:241:VAL:HG11	1:A:290:PHE:HB2	2.03	0.41
1:A:297:ARG:NH2	1:A:1174:ASP:OD2	2.54	0.41
1:A:138:THR:HB	1:A:139:PRO:HD3	2.03	0.41
1:A:808:LYS:HE3	1:A:816:GLN:HB3	2.02	0.41
1:A:848:LEU:HD12	1:A:992:VAL:HG12	2.02	0.41
1:A:829:THR:O	1:A:832:PHE:HB2	2.21	0.40
1:A:153:VAL:HG13	1:A:153:VAL:O	2.21	0.40
1:A:672:ARG:HE	1:A:683:THR:HG21	1.86	0.40
1:A:1001:ARG:HG2	1:A:1092:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	992/1166 (85%)	947 (96%)	41 (4%)	4 (0%)	30	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ASP
1	A	88	VAL
1	A	187	PHE
1	A	699	GLY

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	909/1061 (86%)	887 (98%)	22 (2%)	43	61

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ILE
1	A	177	VAL
1	A	193	HIS
1	A	243	LEU
1	A	263	ASN
1	A	276	THR
1	A	278	ARG
1	A	387	GLN
1	A	435	GLU
1	A	439	ASP
1	A	507	ASP
1	A	660	LEU
1	A	682	ILE

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Mol	Chain	Res	Type
1	A	683	THR
1	A	712	SER
1	A	788	LEU
1	A	968	ARG
1	A	992	VAL
1	A	1064	THR
1	A	1098	LYS
1	A	1112	ILE
1	A	1139	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	149	GLN
1	A	440	GLN
1	A	771	GLN
1	A	868	ASN
1	A	924	GLN
1	A	969	GLN
1	A	1024	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
3	EDO	A	1202	-	3,3,3	0.07	0	2,2,2	0.16	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
3	EDO	A	1202	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	EDO	O1-C1-C2-O2

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	1001/1166 (85%)	0.56	90 (8%) 15 14	27, 56, 107, 151	1 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	839	ILE	5.1
1	A	803	PRO	4.6
1	A	460	PRO	4.4
1	A	638	PRO	4.1
1	A	765	ILE	3.9
1	A	796	ILE	3.9
1	A	190	ILE	3.8
1	A	161	ILE	3.7
1	A	767	PRO	3.6
1	A	281	ALA	3.6
1	A	943	THR	3.5
1	A	475	HIS	3.5
1	A	277	MET	3.4
1	A	205	PHE	3.3
1	A	188	VAL	3.3
1	A	193	HIS	3.2
1	A	818	TYR	3.1
1	A	798	ASN	3.0
1	A	280	THR	3.0
1	A	1188	PRO	3.0
1	A	799	VAL	3.0
1	A	770	PRO	3.0
1	A	1050	PRO	3.0
1	A	909	LYS	3.0
1	A	908	TRP	2.9
1	A	239	SER	2.9
1	A	156	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	788	LEU	2.8
1	A	17	GLN	2.8
1	A	187	PHE	2.8
1	A	772	ARG	2.8
1	A	191	GLY	2.8
1	A	180	ALA	2.8
1	A	1186	MET	2.8
1	A	811	TYR	2.8
1	A	946	ASN	2.8
1	A	837	LYS	2.8
1	A	192	ALA	2.7
1	A	287	VAL	2.7
1	A	840	ILE	2.6
1	A	223	SER	2.6
1	A	181	LYS	2.5
1	A	52	VAL	2.5
1	A	1092	ALA	2.5
1	A	805	GLY	2.5
1	A	61	ILE	2.4
1	A	411	VAL	2.4
1	A	1096	ASN	2.4
1	A	272	PHE	2.4
1	A	178	SER	2.4
1	A	510	GLU	2.4
1	A	179	SER	2.4
1	A	806	TRP	2.4
1	A	89	ARG	2.3
1	A	500	ASP	2.3
1	A	194	LYS	2.3
1	A	813	THR	2.3
1	A	791	CYS	2.3
1	A	1094	TYR	2.3
1	A	282	GLU	2.3
1	A	50	ARG	2.3
1	A	198	SER	2.3
1	A	941	SER	2.3
1	A	243	LEU	2.2
1	A	273	ILE	2.2
1	A	509	ILE	2.2
1	A	1095	ASP	2.2
1	A	834	GLU	2.2
1	A	155	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	763	SER	2.2
1	A	27	VAL	2.2
1	A	942	LYS	2.2
1	A	1125	TYR	2.2
1	A	906	ILE	2.2
1	A	815	ILE	2.1
1	A	242	TYR	2.1
1	A	786	ASP	2.1
1	A	87	ALA	2.1
1	A	266	ARG	2.1
1	A	781	LYS	2.1
1	A	794	ALA	2.1
1	A	218	LEU	2.1
1	A	769	MET	2.0
1	A	257	HIS	2.0
1	A	177	VAL	2.0
1	A	58	ALA	2.0
1	A	200	GLU	2.0
1	A	222	GLY	2.0
1	A	926	ILE	2.0
1	A	678	ASP	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](#)

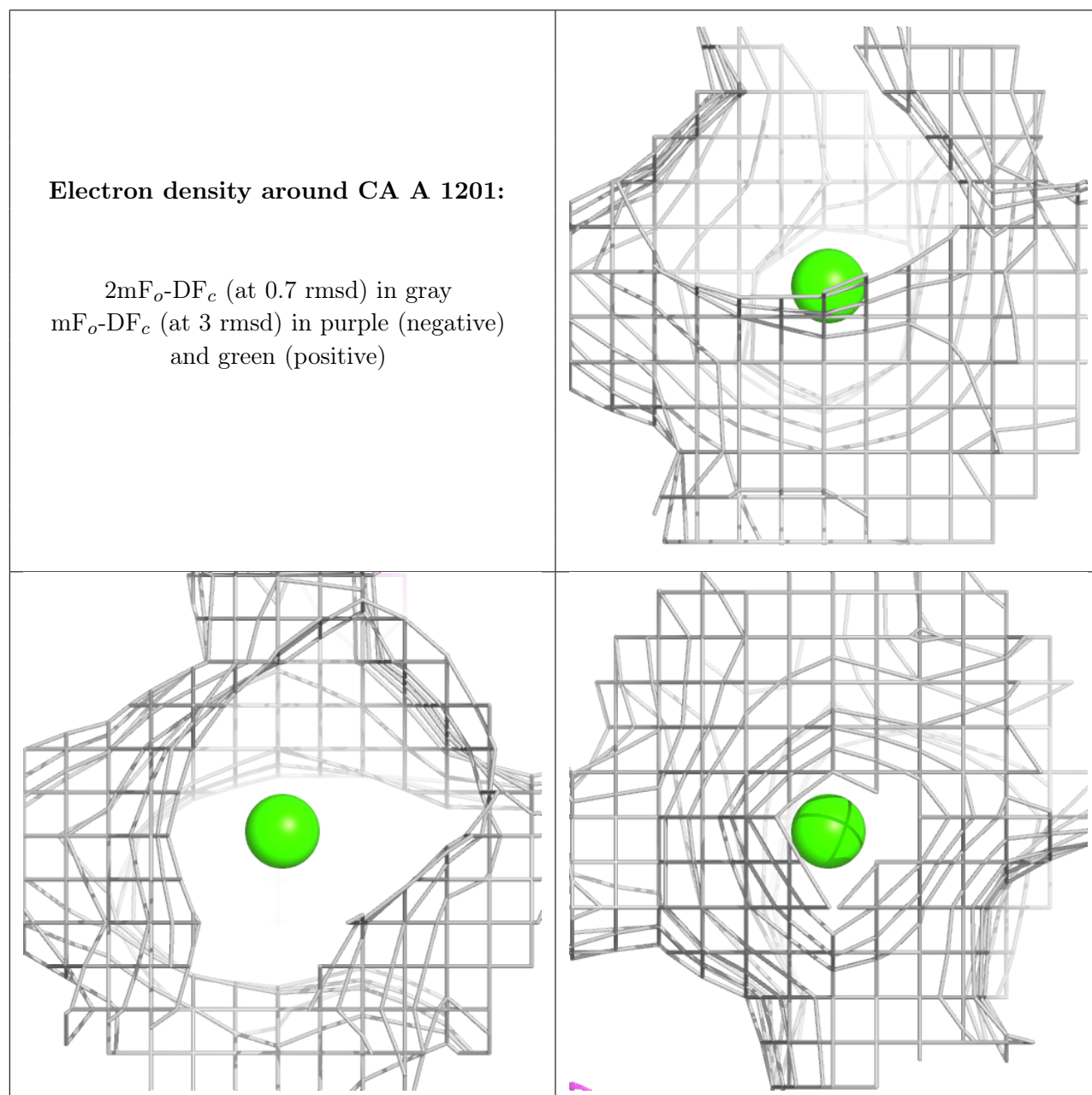
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	EDO	A	1202	4/4	0.93	0.10	51,53,54,56	0
2	CA	A	1201	1/1	0.98	0.04	33,33,33,33	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.