



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:36 AM UTC

PDB ID : 9D16 / pdb\_00009d16  
Title : Tt Pah2 D155N calcium  
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Deposited on : 2024-08-07  
Resolution : 2.40 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](mailto: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>.

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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

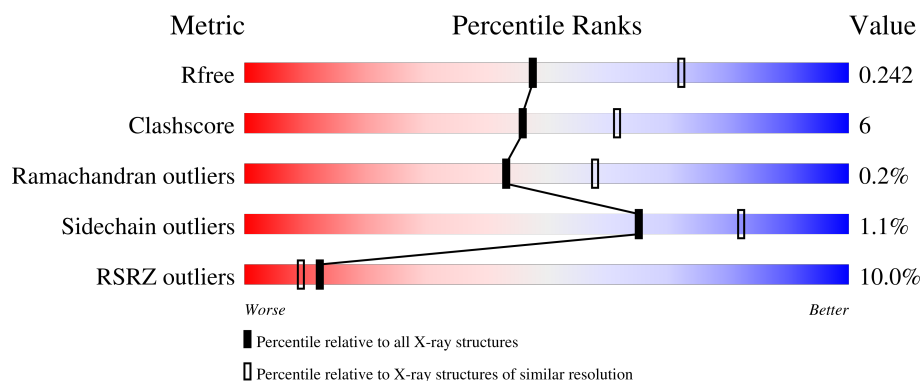
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\geq 3$ , 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	321	<div> <div>8%</div> <div>79%</div> <div>11%</div> <div>11%</div> </div>
1	B	321	<div> <div>10%</div> <div>75%</div> <div>15%</div> <div>9%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9578 atoms, of which 4765 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 Nuclear elongation and deformation protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	H	N	O	S	0	1	0
			4689	1510	2360	376	435	8			
1	B	291	Total	C	H	N	O	S	0	1	0
			4745	1524	2390	383	440	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	ASN	ASP	engineered mutation	UNP I7MFJ3
B	155	ASN	ASP	engineered mutation	UNP I7MFJ3

- 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		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



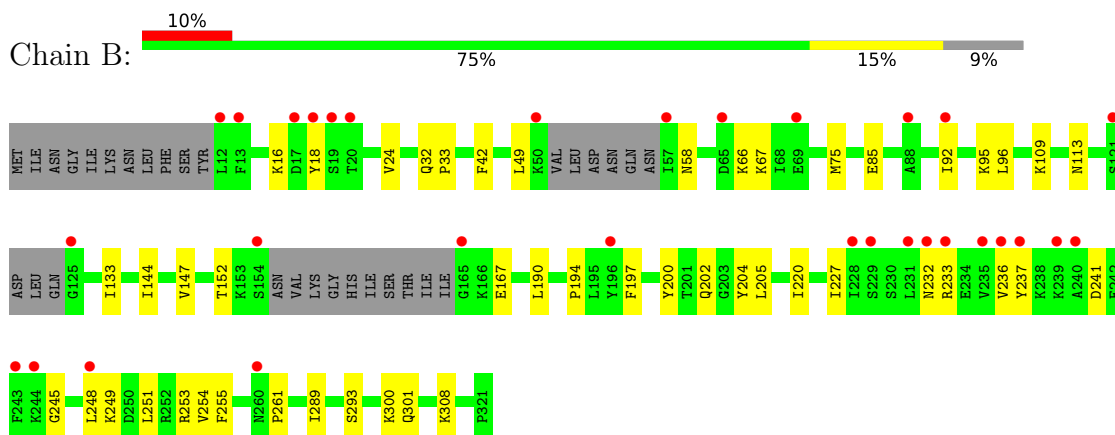
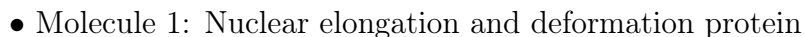
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			13	3	7	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	49	Total	O	0	0
			49	49		



- Molecule 1: Nuclear elongation and deformation protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.28Å 90.04Å 109.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.55 – 2.40 69.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (69.55-2.40) 92.5 (69.55-2.40)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.214 , 0.242 0.214 , 0.242	Depositor DCC
$R_{free}$ test set	1500 reflections (2.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 54.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2940e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, GOL

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	0.21	0/2377	0.35	0/3203
1	B	0.22	0/2403	0.35	0/3237
All	All	0.22	0/4780	0.35	0/6440

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	2329	2360	2357	22	1
1	B	2355	2390	2390	33	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	8	8	0	0
3	B	6	7	8	0	0
4	A	66	0	0	0	0
4	B	49	0	0	6	0
All	All	4813	4765	4763	55	1

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 6.

All (55) 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:B:245:GLY:O	4:B:501:HOH:O	1.76	1.02
1:B:167:GLU:OE2	1:B:200:TYR:OH	1.90	0.87
1:B:245:GLY:O	1:B:249:LYS:HD3	1.83	0.78
1:B:248:LEU:HB2	4:B:501:HOH:O	1.83	0.77
1:B:190:LEU:HD11	1:B:248:LEU:HD21	1.67	0.75
1:A:291:GLU:HG2	1:A:292:GLN:OE1	1.90	0.71
1:A:12:LEU:H	1:A:12:LEU:HD12	1.60	0.66
1:B:249:LYS:CD	4:B:501:HOH:O	2.47	0.61
1:B:251:LEU:O	1:B:254:VAL:HG22	2.01	0.61
1:A:113:ASN:HB2	1:A:133:ILE:HG23	1.83	0.60
1:A:202:GLN:HG2	1:A:220:ILE:HD12	1.86	0.58
1:A:205:LEU:HD12	1:A:220:ILE:HD11	1.84	0.58
1:B:232:ASN:OD1	1:B:236:VAL:HG21	2.05	0.57
1:B:205:LEU:HD12	1:B:220:ILE:HD11	1.87	0.56
1:B:249:LYS:HD3	4:B:501:HOH:O	2.05	0.56
1:B:16:LYS:HB2	1:B:18:TYR:CE2	2.41	0.56
1:A:62:THR:HG23	1:A:66:LYS:C	2.32	0.54
1:A:24:VAL:CG2	1:A:131:GLY:HA3	2.38	0.53
1:B:249:LYS:N	1:B:249:LYS:HD2	2.24	0.53
1:A:24:VAL:HG21	1:A:131:GLY:HA3	1.92	0.52
1:A:60:GLN:HG3	1:A:120:GLU:OE2	2.11	0.50
1:B:113:ASN:HB2	1:B:133:ILE:HG23	1.93	0.50
1:B:249:LYS:O	1:B:253:ARG:HG3	2.11	0.50
1:A:49:LEU:HD23	1:A:75:MET:HE1	1.95	0.48
1:B:152:THR:HG22	1:B:204:TYR:OH	2.14	0.48
1:B:66:LYS:NZ	1:B:67:LYS:O	2.46	0.48
1:B:289:ILE:HD11	1:B:293:SER:HA	1.94	0.47
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.79	0.47
1:A:76:LEU:CD1	1:A:231:LEU:HD11	2.45	0.47
1:B:16:LYS:HB2	1:B:18:TYR:CD2	2.50	0.47
1:B:194:PRO:HD2	1:B:197:PHE:HD2	1.79	0.47
1:B:58:ASN:OD1	1:B:58:ASN:C	2.58	0.47
1:B:109:LYS:NZ	4:B:505:HOH:O	2.44	0.46
1:A:178:THR:O	1:A:182:LYS:HG3	2.15	0.46
1:B:49:LEU:HD22	1:B:75:MET:HE1	1.97	0.46
1:A:228:ILE:HD11	1:A:236:VAL:CG1	2.45	0.46
1:A:97:ARG:CZ	1:A:253:ARG:NH2	2.79	0.45
1:B:147:VAL:HG23	1:B:190:LEU:O	2.16	0.45
1:B:16:LYS:HD2	1:B:18:TYR:HE2	1.81	0.45
1:A:96:LEU:HD21	1:A:231:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:SER:O	1:A:233:ARG:HG3	2.17	0.45
1:B:32:GLN:HB3	1:B:33:PRO:HD2	1.99	0.44
1:A:230:SER:HA	1:A:233:ARG:NE	2.33	0.44
1:B:227:ILE:C	1:B:227:ILE:HD12	2.43	0.43
1:A:204:TYR:CZ	1:A:208:ILE:HD11	2.54	0.43
1:B:202:GLN:HG2	1:B:220:ILE:HD12	2.00	0.43
1:A:121:SER:OG	1:A:125:GLY:N	2.52	0.43
1:B:300:LYS:O	1:B:301:GLN:C	2.62	0.42
1:B:85:GLU:OE1	1:B:95:LYS:HD2	2.19	0.42
1:B:249:LYS:CD	1:B:249:LYS:N	2.81	0.42
1:B:255:PHE:CD1	1:B:261:PRO:HG3	2.54	0.42
1:B:42:PHE:O	1:B:96:LEU:HD22	2.20	0.41
1:A:121:SER:HG	1:A:125:GLY:N	2.18	0.41
1:A:24:VAL:HG12	1:A:44:ILE:HB	2.03	0.41
1:B:245:GLY:HA2	4:B:501:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TYR:OH	1:B:233:ARG:HH12[1_655]	1.47	0.13

## 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	278/321 (87%)	268 (96%)	10 (4%)	0	100	100
1	B	284/321 (88%)	266 (94%)	17 (6%)	1 (0%)	30	43
All	All	562/642 (88%)	534 (95%)	27 (5%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	ILE

### 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	261/290 (90%)	260 (100%)	1 (0%)	84	92
1	B	263/290 (91%)	258 (98%)	5 (2%)	50	71
All	All	524/580 (90%)	518 (99%)	6 (1%)	65	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	SER
1	B	24	VAL
1	B	144	ILE
1	B	237	TYR
1	B	241	ASP
1	B	308	LYS

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	127	GLN
1	A	260	ASN
1	A	294	GLN
1	B	107	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	GOL	B	401	-	5,5,5	0.92	0	5,5,5	1.26	1 (20%)
3	GOL	A	401	-	5,5,5	0.73	0	5,5,5	1.13	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	GOL	B	401	-	-	0/4/4/4	-
3	GOL	A	401	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	GOL	C3-C2-C1	-2.23	103.61	111.80

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	287/321 (89%)	0.57	27 (9%) 14 11	35, 68, 137, 171	1 (0%)
1	B	291/321 (90%)	0.68	31 (10%) 11 8	42, 73, 133, 173	1 (0%)
All	All	578/642 (90%)	0.62	58 (10%) 12 9	35, 71, 137, 173	2 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	PHE	5.5
1	B	236	VAL	4.5
1	A	236	VAL	4.2
1	A	18	TYR	4.0
1	B	88	ALA	3.9
1	A	235	VAL	3.8
1	B	121	SER	3.5
1	A	240	ALA	3.5
1	A	237	TYR	3.5
1	B	154	SER	3.4
1	A	232	ASN	3.4
1	A	10	SER	3.4
1	B	18	TYR	3.3
1	B	20	THR	3.3
1	A	11	TYR	3.2
1	B	237	TYR	3.2
1	B	12	LEU	3.2
1	A	229	SER	3.1
1	B	92	ILE	3.0
1	B	235	VAL	3.0
1	A	19	SER	3.0
1	A	13	PHE	3.0
1	A	154	SER	2.9
1	A	49	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	125	GLY	2.8
1	A	14	ASP	2.8
1	A	92	ILE	2.8
1	B	19	SER	2.7
1	A	48	THR	2.7
1	B	125	GLY	2.7
1	B	50	LYS	2.7
1	B	243	PHE	2.6
1	A	87	ASN	2.6
1	B	17	ASP	2.6
1	A	239	LYS	2.6
1	A	12	LEU	2.6
1	B	228	ILE	2.5
1	A	270	ASP	2.5
1	A	168	TRP	2.4
1	A	47	GLY	2.4
1	B	57	ILE	2.4
1	B	240	ALA	2.4
1	B	233	ARG	2.3
1	B	248	LEU	2.3
1	A	241	ASP	2.3
1	B	239	LYS	2.3
1	B	260	ASN	2.3
1	B	69	GLU	2.3
1	B	231	LEU	2.2
1	B	65	ASP	2.2
1	A	243	PHE	2.2
1	B	196	TYR	2.1
1	A	20	THR	2.1
1	B	244	LYS	2.1
1	B	165	GLY	2.1
1	B	229	SER	2.1
1	A	208	ILE	2.1
1	B	232	ASN	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](#)

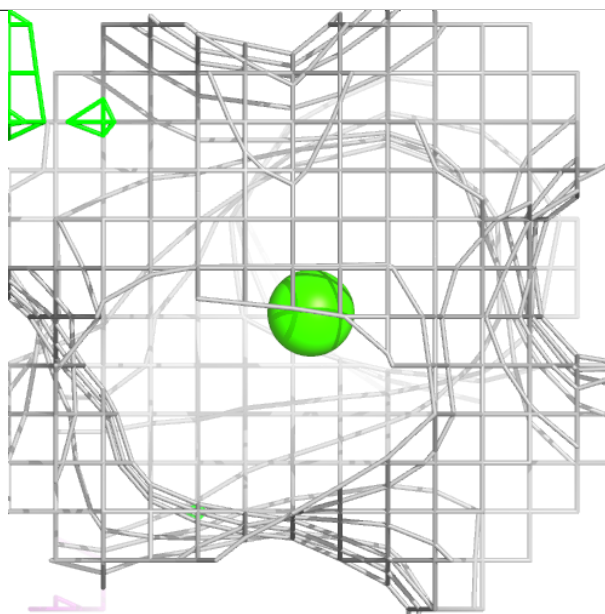
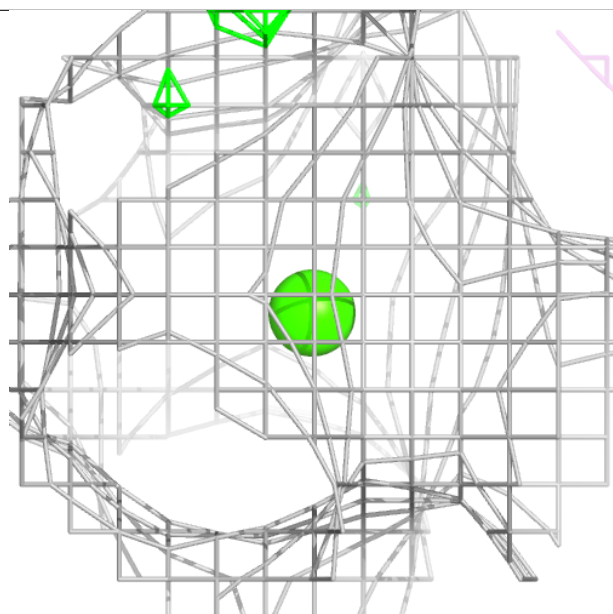
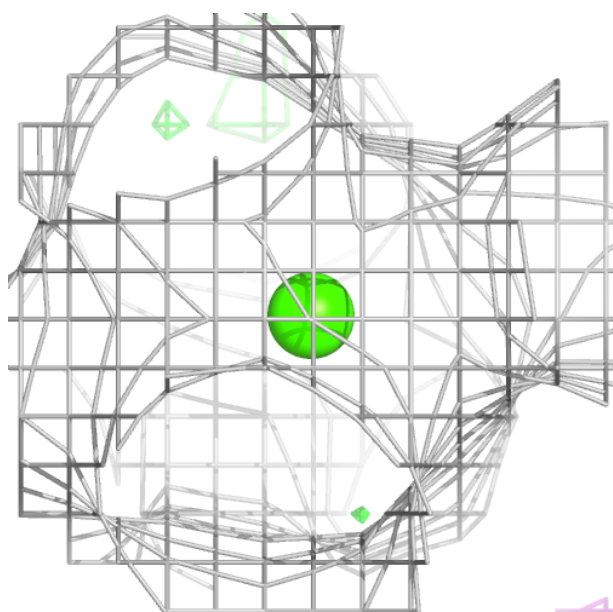
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	GOL	B	401	6/6	0.92	0.14	60,69,78,83	0
3	GOL	A	401	6/6	0.95	0.09	55,68,75,82	0
2	CA	B	400	1/1	0.96	0.05	64,64,64,64	0
2	CA	A	400	1/1	0.97	0.05	64,64,64,64	0

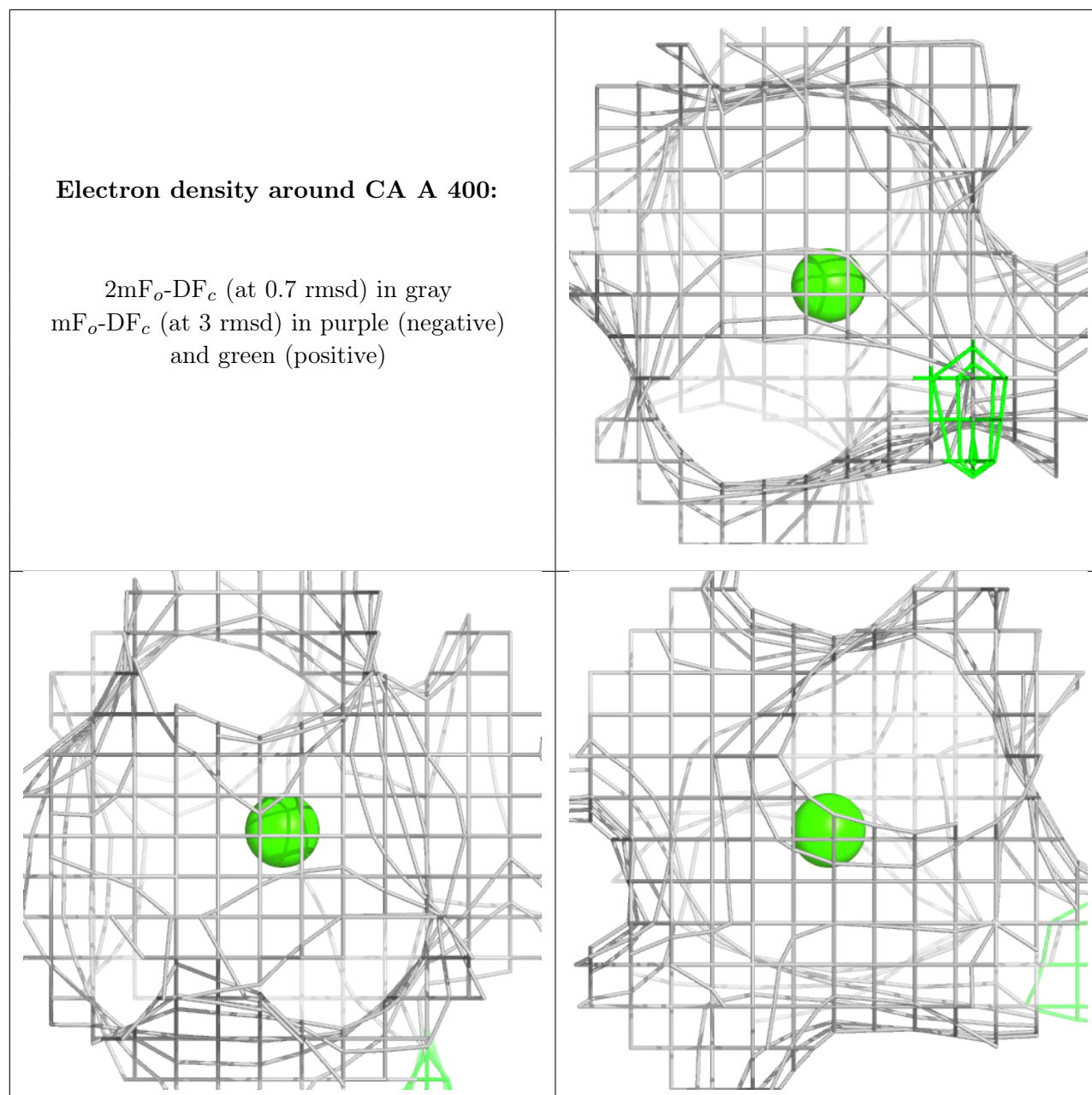
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around CA B 400:**

$2mF_o-DF_c$  (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.