



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:46 PM UTC

PDB ID : 7Z4Q / pdb_00007z4q
Title : Plasmodium falciparum pyruvate kinase mutant - C49A
Authors : Dillenberger, M.; Rahlfs, S.; Becker, K.; Fritz-Wolf, K.
Deposited on : 2022-03-04
Resolution : 2.10 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

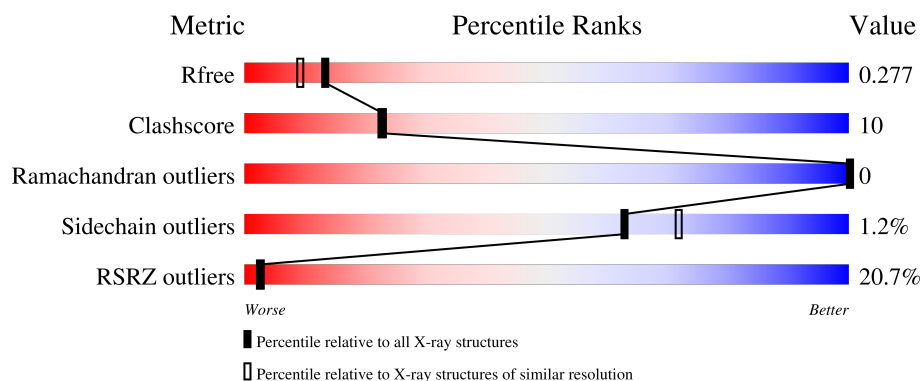
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	519	20% 73% 23% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3836 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3781	2381	653	718	29			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	ALA	CYS	engineered mutation	UNP C6KTA4
A	512	LEU	-	expression tag	UNP C6KTA4
A	513	GLU	-	expression tag	UNP C6KTA4
A	514	HIS	-	expression tag	UNP C6KTA4
A	515	HIS	-	expression tag	UNP C6KTA4
A	516	HIS	-	expression tag	UNP C6KTA4
A	517	HIS	-	expression tag	UNP C6KTA4
A	518	HIS	-	expression tag	UNP C6KTA4
A	519	HIS	-	expression tag	UNP C6KTA4

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	89.66Å 109.81Å 133.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.20 – 2.10 41.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (41.20-2.10) 98.6 (41.20-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.251 , 0.278 0.251 , 0.277	Depositor DCC
R_{free} test set	3058 reflections (8.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	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	0.95	EDS
Total number of atoms	3836	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: MG

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	0.12	0/3826	0.32	0/5164

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 [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	3781	0	3941	80	0
2	A	1	0	0	0	0
3	A	54	0	0	4	0
All	All	3836	0	3941	80	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 10.

All (80) 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:77:ASP:HA	1:A:80:GLU:HB3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HD11	1:A:309:ILE:HD11	1.68	0.76
1:A:264:HIS:HB3	1:A:267:LYS:HE3	1.66	0.75
1:A:436:LEU:HD11	1:A:457:ILE:HD12	1.69	0.74
1:A:50:LYS:HE3	1:A:81:MET:HA	1.70	0.74
1:A:210:LYS:HD2	1:A:242:LEU:HD23	1.70	0.73
1:A:422:THR:HG23	1:A:494:ILE:HD12	1.74	0.69
1:A:504:LEU:HD21	1:A:506:LYS:HG3	1.79	0.65
1:A:83:ASN:O	1:A:87:LYS:HG2	1.96	0.64
1:A:50:LYS:HD3	1:A:50:LYS:O	1.98	0.64
1:A:268:ILE:O	1:A:272:SER:OG	2.15	0.62
1:A:417:THR:HB	1:A:422:THR:HB	1.81	0.62
1:A:233:ALA:H	1:A:267:LYS:HZ1	1.46	0.61
1:A:279:ARG:NH1	1:A:350:THR:HG21	2.14	0.61
1:A:388:GLU:HB3	1:A:390:PRO:HD2	1.83	0.60
1:A:106:PRO:HB3	1:A:202:LEU:HB2	1.86	0.58
1:A:314:GLN:NE2	3:A:704:HOH:O	2.32	0.57
1:A:51:SER:O	1:A:54:THR:N	2.38	0.56
1:A:59:ILE:HD11	1:A:97:LEU:HD11	1.87	0.56
1:A:279:ARG:HH11	1:A:314:GLN:HG2	1.71	0.54
1:A:323:PRO:HG3	1:A:355:PHE:CE1	2.42	0.54
1:A:58:LEU:HB3	1:A:63:MET:HE2	1.90	0.53
1:A:79:LYS:HA	1:A:82:PHE:HD1	1.73	0.53
1:A:113:LEU:HB2	1:A:116:LYS:HA	1.91	0.52
1:A:225:ILE:HD12	1:A:243:LEU:HD21	1.90	0.52
1:A:106:PRO:HG2	1:A:229:PHE:HB3	1.92	0.51
1:A:377:LYS:O	1:A:381:GLN:HG3	2.11	0.51
1:A:494:ILE:HG12	1:A:503:ASN:OD1	2.10	0.51
1:A:170:LEU:HD11	1:A:180:GLU:HB2	1.92	0.51
1:A:213:ILE:HA	1:A:217:ALA:HB3	1.93	0.50
1:A:233:ALA:H	1:A:267:LYS:NZ	2.08	0.50
1:A:470:ARG:HA	1:A:473:ILE:HB	1.95	0.49
1:A:346:LEU:HG	1:A:363:MET:SD	2.53	0.49
1:A:279:ARG:CZ	1:A:350:THR:HG21	2.43	0.48
1:A:424:ARG:NH1	3:A:707:HOH:O	2.45	0.48
1:A:234:ASP:OD1	1:A:237:ARG:NH2	2.45	0.48
1:A:161:ALA:O	1:A:164:SER:OG	2.31	0.48
1:A:116:LYS:HG2	1:A:189:GLU:CD	2.39	0.47
1:A:160:ILE:HB	1:A:165:VAL:HG23	1.97	0.46
1:A:257:GLU:HB3	1:A:281:ASP:HB2	1.97	0.46
1:A:383:LEU:HD11	1:A:430:LYS:HD2	1.97	0.46
1:A:379:LEU:HD21	1:A:430:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLN:OE1	1:A:16:GLN:HA	2.14	0.46
1:A:40:HIS:ND1	1:A:449:ASN:O	2.48	0.46
1:A:500:GLY:HA2	1:A:501:GLY:HA3	1.62	0.46
1:A:346:LEU:HD11	1:A:359:ALA:HB3	1.97	0.46
1:A:50:LYS:CE	1:A:81:MET:HA	2.44	0.45
1:A:448:LEU:HB2	1:A:456:CYS:SG	2.57	0.45
1:A:44:THR:HG23	1:A:67:ARG:HG2	1.99	0.45
1:A:89:GLN:NE2	1:A:97:LEU:H	2.15	0.45
1:A:165:VAL:HG13	1:A:185:ALA:HB3	1.99	0.45
1:A:491:ILE:HD11	1:A:494:ILE:HD11	2.00	0.44
1:A:74:SER:HG	1:A:77:ASP:H	1.64	0.44
1:A:233:ALA:HB1	1:A:271:GLU:HG3	1.99	0.44
1:A:492:HIS:NE2	1:A:504:LEU:HD22	2.32	0.44
1:A:279:ARG:NH1	1:A:314:GLN:HA	2.33	0.44
1:A:279:ARG:HE	1:A:312:ALA:HB1	1.82	0.44
1:A:315:MET:HE3	1:A:316:LEU:HG	2.00	0.44
1:A:276:MET:HE2	1:A:345:MET:SD	2.57	0.44
1:A:71:SER:HB3	1:A:72:HIS:CE1	2.53	0.44
1:A:157:ILE:O	1:A:196:PRO:HD2	2.18	0.43
1:A:350:THR:C	1:A:352:GLY:H	2.25	0.43
1:A:397:VAL:HG21	1:A:503:ASN:HB3	2.01	0.43
1:A:457:ILE:HD13	1:A:475:ILE:HD11	2.00	0.43
1:A:239:ILE:O	1:A:243:LEU:HD13	2.18	0.43
1:A:246:ARG:H	1:A:246:ARG:HG3	1.67	0.43
1:A:216:PHE:C	1:A:219:PRO:HD2	2.43	0.43
1:A:259:ILE:O	1:A:263:ILE:HG13	2.19	0.42
1:A:327:ARG:O	1:A:331:THR:HG23	2.19	0.42
1:A:15:MET:SD	1:A:296:LYS:HB3	2.60	0.42
1:A:51:SER:O	1:A:55:LEU:HD12	2.19	0.41
1:A:352:GLY:C	1:A:354:LYS:H	2.29	0.41
1:A:53:GLU:H	1:A:53:GLU:CD	2.29	0.41
1:A:470:ARG:HH12	1:A:511:GLU:H	1.68	0.41
1:A:74:SER:OG	1:A:77:ASP:OD1	2.29	0.41
1:A:323:PRO:HG3	1:A:355:PHE:CD1	2.56	0.41
1:A:171:GLU:HB2	1:A:178:ILE:HB	2.03	0.40
1:A:428:LYS:NZ	3:A:714:HOH:O	2.53	0.40
1:A:319:MET:SD	1:A:319:MET:N	2.95	0.40
1:A:339:ASP:OD1	3:A:701:HOH:O	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	493/519 (95%)	478 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	426/445 (96%)	421 (99%)	5 (1%)	63	72

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	51	SER
1	A	109	ARG
1	A	206	SER
1	A	347	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	264	HIS
1	A	303	ASN

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Mol	Chain	Res	Type
1	A	385	ASN
1	A	451	HIS
1	A	463	GLN
1	A	503	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 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	497/519 (95%)	1.32	103 (20%) 2 3	45, 70, 110, 144	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	LEU	6.6
1	A	350	THR	6.1
1	A	49	ALA	5.7
1	A	243	LEU	5.6
1	A	242	LEU	5.1
1	A	494	ILE	5.0
1	A	502	THR	4.9
1	A	351	ALA	4.8
1	A	278	ALA	4.5
1	A	70	PHE	4.4
1	A	13	ALA	4.4
1	A	316	LEU	4.4
1	A	277	ILE	4.3
1	A	355	PHE	4.2
1	A	352	GLY	4.2
1	A	216	PHE	4.2
1	A	495	LYS	4.1
1	A	214	LEU	4.1
1	A	389	THR	3.7
1	A	47	PRO	3.7
1	A	218	ILE	3.7
1	A	279	ARG	3.5
1	A	501	GLY	3.5
1	A	82	PHE	3.4
1	A	95	CYS	3.4
1	A	85	VAL	3.4
1	A	135	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	210	LYS	3.3
1	A	353	GLY	3.3
1	A	500	GLY	3.3
1	A	508	VAL	3.2
1	A	475	ILE	3.1
1	A	15	MET	3.1
1	A	315	MET	3.1
1	A	244	GLY	3.0
1	A	105	GLY	3.0
1	A	320	THR	3.0
1	A	390	PRO	3.0
1	A	346	LEU	2.9
1	A	81	MET	2.9
1	A	27	LEU	2.9
1	A	166	SER	2.9
1	A	48	ALA	2.8
1	A	71	SER	2.8
1	A	493	GLY	2.8
1	A	238	LEU	2.8
1	A	204	ILE	2.8
1	A	16	GLN	2.8
1	A	314	GLN	2.8
1	A	503	ASN	2.7
1	A	17	SER	2.7
1	A	165	VAL	2.7
1	A	286	ILE	2.7
1	A	360	VAL	2.7
1	A	323	PRO	2.6
1	A	470	ARG	2.6
1	A	46	GLY	2.6
1	A	86	LEU	2.6
1	A	159	LEU	2.6
1	A	462	PHE	2.5
1	A	327	ARG	2.5
1	A	250	ILE	2.5
1	A	347	SER	2.5
1	A	83	ASN	2.5
1	A	349	GLU	2.4
1	A	184	SER	2.4
1	A	45	LEU	2.4
1	A	104	LYS	2.4
1	A	262	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	318	SER	2.4
1	A	312	ALA	2.4
1	A	170	LEU	2.4
1	A	213	ILE	2.4
1	A	247	GLY	2.3
1	A	221	GLY	2.3
1	A	31	ASN	2.3
1	A	206	SER	2.3
1	A	68	PHE	2.2
1	A	313	THR	2.2
1	A	63	MET	2.2
1	A	23	LEU	2.2
1	A	55	LEU	2.2
1	A	354	LYS	2.2
1	A	20	ASN	2.2
1	A	276	MET	2.2
1	A	457	ILE	2.2
1	A	119	HIS	2.1
1	A	267	LYS	2.1
1	A	249	HIS	2.1
1	A	79	LYS	2.1
1	A	96	LEU	2.1
1	A	385	ASN	2.1
1	A	245	PRO	2.1
1	A	186	VAL	2.1
1	A	215	ASN	2.1
1	A	449	ASN	2.1
1	A	52	VAL	2.1
1	A	282	LEU	2.0
1	A	239	ILE	2.0
1	A	291	VAL	2.0
1	A	284	MET	2.0
1	A	69	ASN	2.0
1	A	373	CYS	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](#)

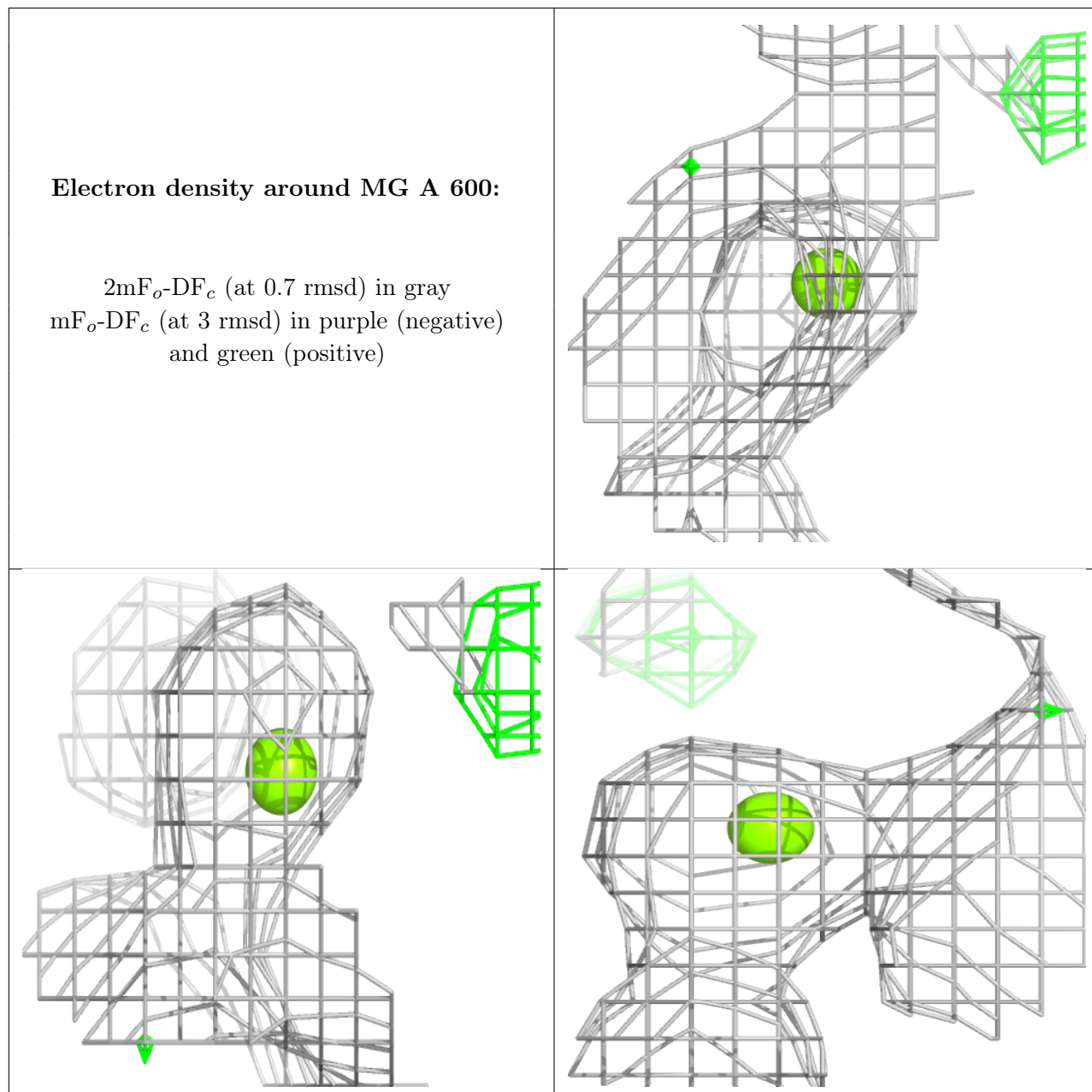
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	A	600	1/1	0.92	0.13	70,70,70,70	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 MG A 600:

$2mF_o-DF_c$ (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.