Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 01:46 AM EDT

PDB ID	:	6V9K / pdb_00006v9k
Title	:	CRYSTAL STRUCTURE OF THE HYBRID C-TERMINAL DOMAIN OF ENZYME I OF THE BACTERIAL PHOSPHOTRANSFERASE SYSTEM FORMED BY HYBRIDIZING THE SCAFFOLD OF THE ESCHERICHIA COLI ENZYME WITH THE ACTIVE SITE LOOPS FROM THE THERMOANAEROBACTER TENGCONGENSIS ENZYME
Authors	:	Stewart Jr., C.E.
Deposited on	:	2019-12-13
Resolution	:	1.90 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:

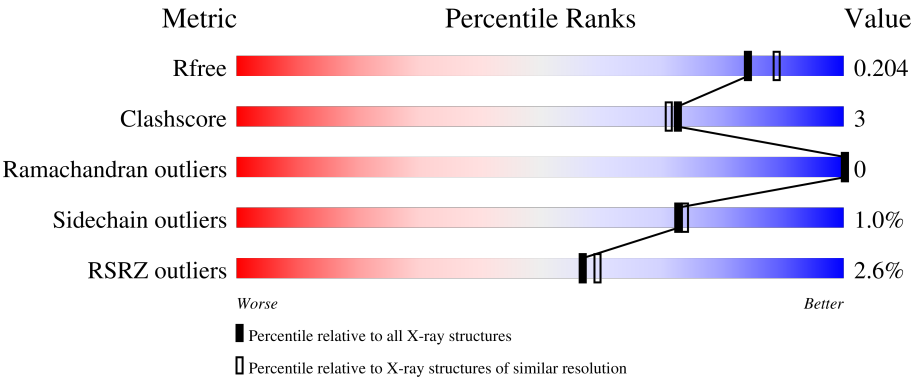
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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 <=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	316	3% 91% 7%
1	B	316	2% 91% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10416 atoms, of which 4929 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 Phosphoenolpyruvate-protein phosphotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	310	Total	C	H	N	O	S	0	4	0
			4956	1563	2483	422	472	16			
1	B	310	Total	C	H	N	O	S	0	0	0
			4880	1538	2446	415	466	15			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	MET	-	initiating methionine	UNP A0A4S4CN20
A	278	PRO	VAL	engineered mutation	UNP A0A4S4CN20
A	279	LYS	ARG	engineered mutation	UNP A0A4S4CN20
A	301	TYR	PHE	engineered mutation	UNP A0A4S4CN20
A	305	ASN	ASP	engineered mutation	UNP A0A4S4CN20
A	306	SER	ALA	engineered mutation	UNP A0A4S4CN20
A	309	SER	THR	engineered mutation	UNP A0A4S4CN20
A	334	LEU	MET	engineered mutation	UNP A0A4S4CN20
A	345	LEU	MET	engineered mutation	UNP A0A4S4CN20
A	346	ASP	ASN	engineered mutation	UNP A0A4S4CN20
A	347	MET	PHE	engineered mutation	UNP A0A4S4CN20
A	351	MET	GLU	engineered mutation	UNP A0A4S4CN20
A	357	TYR	TRP	engineered mutation	UNP A0A4S4CN20
A	466	MET	GLY	engineered mutation	UNP A0A4S4CN20
A	468	GLU	ASP	engineered mutation	UNP A0A4S4CN20
A	469	HIS	MET	engineered mutation	UNP A0A4S4CN20
A	470	VAL	ILE	engineered mutation	UNP A0A4S4CN20
A	471	LYS	SER	engineered mutation	UNP A0A4S4CN20
A	472	GLU	HIS	engineered mutation	UNP A0A4S4CN20
A	473	TYR	LEU	engineered mutation	UNP A0A4S4CN20
A	477	PHE	MET	engineered mutation	UNP A0A4S4CN20
A	478	HIS	SER	engineered mutation	UNP A0A4S4CN20
B	260	MET	-	initiating methionine	UNP A0A4S4CN20
B	278	PRO	VAL	engineered mutation	UNP A0A4S4CN20
B	279	LYS	ARG	engineered mutation	UNP A0A4S4CN20

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Chain	Residue	Modelled	Actual	Comment	Reference
B	301	TYR	PHE	engineered mutation	UNP A0A4S4CN20
B	305	ASN	ASP	engineered mutation	UNP A0A4S4CN20
B	306	SER	ALA	engineered mutation	UNP A0A4S4CN20
B	309	SER	THR	engineered mutation	UNP A0A4S4CN20
B	334	LEU	MET	engineered mutation	UNP A0A4S4CN20
B	345	LEU	MET	engineered mutation	UNP A0A4S4CN20
B	346	ASP	ASN	engineered mutation	UNP A0A4S4CN20
B	347	MET	PHE	engineered mutation	UNP A0A4S4CN20
B	351	MET	GLU	engineered mutation	UNP A0A4S4CN20
B	357	TYR	TRP	engineered mutation	UNP A0A4S4CN20
B	466	MET	GLY	engineered mutation	UNP A0A4S4CN20
B	468	GLU	ASP	engineered mutation	UNP A0A4S4CN20
B	469	HIS	MET	engineered mutation	UNP A0A4S4CN20
B	470	VAL	ILE	engineered mutation	UNP A0A4S4CN20
B	471	LYS	SER	engineered mutation	UNP A0A4S4CN20
B	472	GLU	HIS	engineered mutation	UNP A0A4S4CN20
B	473	TYR	LEU	engineered mutation	UNP A0A4S4CN20
B	477	PHE	MET	engineered mutation	UNP A0A4S4CN20
B	478	HIS	SER	engineered mutation	UNP A0A4S4CN20

- 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 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is water.

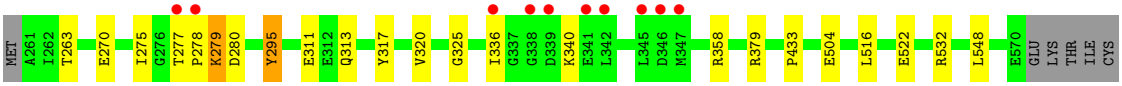
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	279	Total O 279 279	0	0
3	B	299	Total O 299 299	0	0

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.

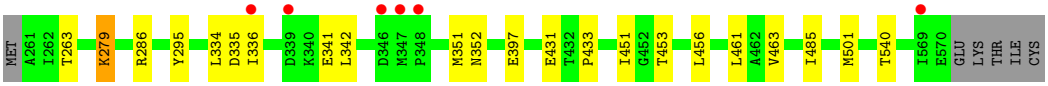
• Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

Chain A:



• Molecule 1: Phosphoenolpyruvate-protein phosphotransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.38Å 69.53Å 84.66Å 90.00° 108.73° 90.00°	Depositor
Resolution (Å)	42.81 – 1.90 42.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (42.81-1.90) 98.8 (42.81-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.14.3260	Depositor
R, R_{free}	0.161 , 0.204 0.162 , 0.204	Depositor DCC
R_{free} test set	2503 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10416	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.44	0/2512	0.54	0/3387
1	B	0.47	0/2472	0.55	0/3334
All	All	0.46	0/4984	0.55	0/6721

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	2473	2483	2480	15	2
1	B	2434	2446	2446	16	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	279	0	0	4	2
3	B	299	0	0	3	2
All	All	5487	4929	4926	30	4

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 3.

All (30) 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:358[A]:ARG:NH1	3:A:701:HOH:O	2.08	0.85
1:A:532:ARG:NH1	3:A:702:HOH:O	2.14	0.80
1:B:336:ILE:HD11	1:B:341:GLU:HB3	1.68	0.76
1:A:336:ILE:HD11	1:A:340:LYS:HG3	1.71	0.70
1:B:451:ILE:HD13	1:B:485:ILE:HG23	1.73	0.70
1:A:275:ILE:HG23	1:A:280:ASP:HB2	1.75	0.68
1:B:397:GLU:OE1	3:B:701:HOH:O	2.13	0.67
1:A:295:TYR:CE2	1:A:320:VAL:HG11	2.35	0.61
1:B:334:LEU:HD11	1:B:336:ILE:HG22	1.81	0.61
1:B:335:ASP:OD1	3:B:702:HOH:O	2.18	0.57
1:B:351:MET:HG2	1:B:352:ASN:ND2	2.20	0.57
1:B:334:LEU:CD1	1:B:336:ILE:HG22	2.41	0.51
1:A:277:THR:HG21	1:A:279:LYS:HD3	1.92	0.51
1:A:311:GLU:OE1	1:A:379:ARG:NH2	2.36	0.50
1:B:334:LEU:HD11	1:B:336:ILE:CG2	2.42	0.50
1:B:341:GLU:OE1	1:B:341:GLU:N	2.44	0.49
1:A:270[B]:GLU:OE2	3:A:703:HOH:O	2.20	0.47
1:B:336:ILE:HG23	1:B:342:LEU:HD11	1.97	0.47
1:B:286:ARG:NH2	3:B:705:HOH:O	2.33	0.46
1:A:548:LEU:C	1:A:548:LEU:HD13	2.35	0.46
1:B:461:LEU:HB2	1:B:463:VAL:HG12	1.99	0.45
1:B:263:THR:HB	1:B:540:THR:O	2.18	0.44
1:A:295:TYR:CD2	1:A:320:VAL:HG11	2.54	0.43
1:A:325:GLY:O	3:A:704:HOH:O	2.22	0.42
1:A:277:THR:OG1	1:A:278:PRO:CD	2.68	0.42
1:A:433:PRO:HG2	1:B:433:PRO:HG2	2.02	0.41
1:B:453:THR:HG21	1:B:501:MET:SD	2.60	0.41
1:A:313:GLN:HB3	1:A:317:TYR:CE2	2.56	0.41
1:A:263:THR:HG22	1:A:516:LEU:HD21	2.02	0.40
1:B:431:GLU:O	1:B:456:LEU:HA	2.21	0.40

All (4) 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:504:GLU:OE2	1:B:279:LYS:NZ[2_656]	2.11	0.09
3:A:915:HOH:O	3:B:872:HOH:O[1_454]	2.12	0.08
3:A:915:HOH:O	3:B:831:HOH:O[1_454]	2.14	0.06
1:A:504:GLU:OE2	1:B:279:LYS:HZ1[2_656]	1.59	0.01

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	312/316 (99%)	308 (99%)	4 (1%)	0	100	100
1	B	308/316 (98%)	300 (97%)	8 (3%)	0	100	100
All	All	620/632 (98%)	608 (98%)	12 (2%)	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	262/264 (99%)	259 (99%)	3 (1%)	70	71
1	B	258/264 (98%)	256 (99%)	2 (1%)	79	80
All	All	520/528 (98%)	515 (99%)	5 (1%)	73	74

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

Mol	Chain	Res	Type
1	A	279	LYS
1	A	295	TYR
1	A	522	GLU
1	B	279	LYS
1	B	295	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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^{th} 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	310/316 (98%)	-0.32	10 (3%) 50 52	10, 24, 55, 79	4 (1%)
1	B	310/316 (98%)	-0.46	6 (1%) 66 68	12, 21, 50, 78	0
All	All	620/632 (98%)	-0.39	16 (2%) 57 59	10, 23, 53, 79	4 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	ASP	3.5
1	A	342	LEU	3.4
1	A	277	THR	3.2
1	A	345	LEU	3.2
1	A	347[A]	MET	2.8
1	B	339	ASP	2.7
1	A	278	PRO	2.5
1	B	346	ASP	2.5
1	A	338	GLY	2.2
1	A	336	ILE	2.2
1	B	569	ILE	2.2
1	B	348	PRO	2.1
1	A	346	ASP	2.1
1	A	341	GLU	2.1
1	B	347	MET	2.1
1	B	336	ILE	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 monosaccharides in this entry.

6.4 Ligands (i)

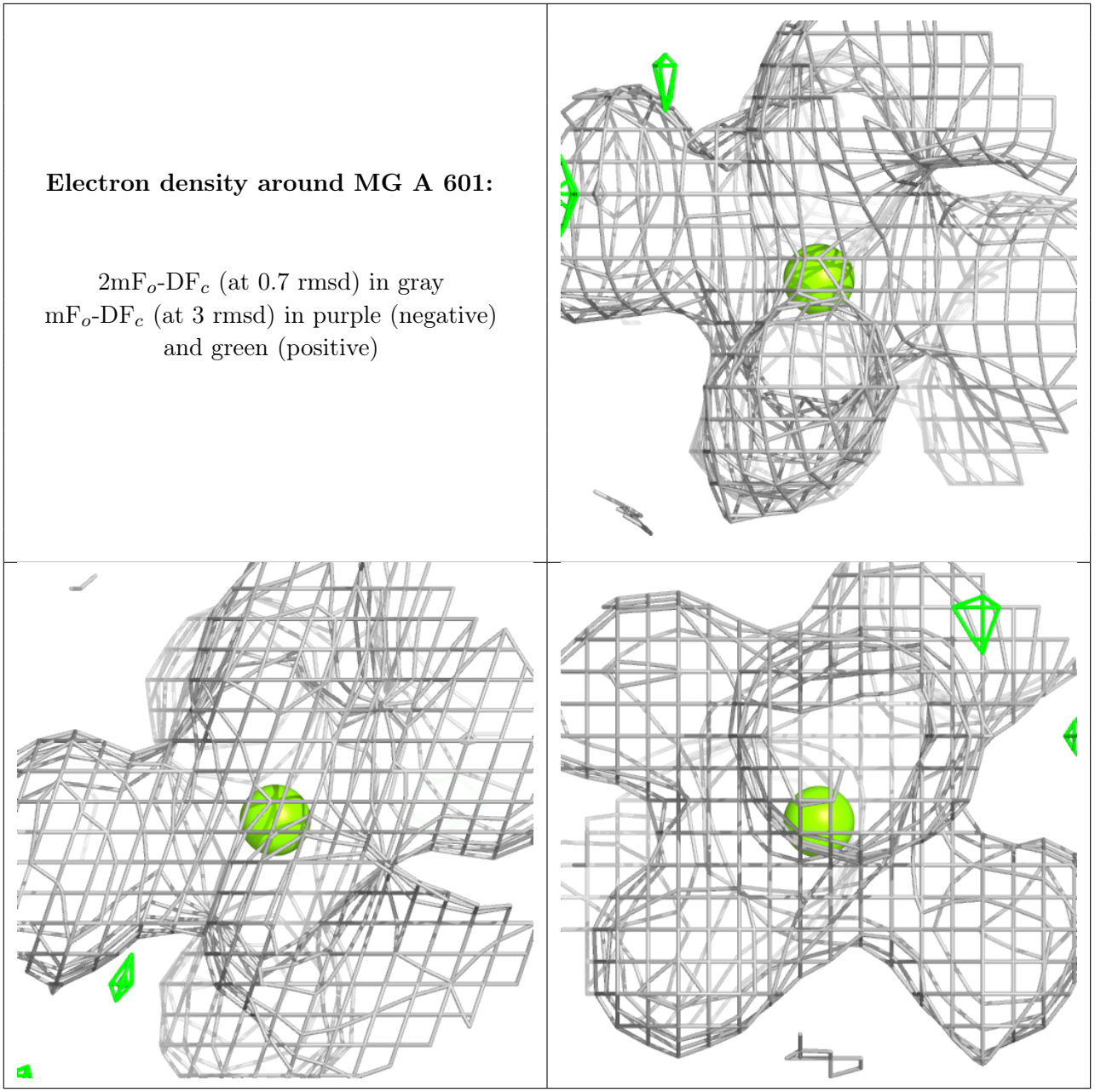
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	601	1/1	0.95	0.06	36,36,36,36	0
2	MG	B	601	1/1	0.98	0.07	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.

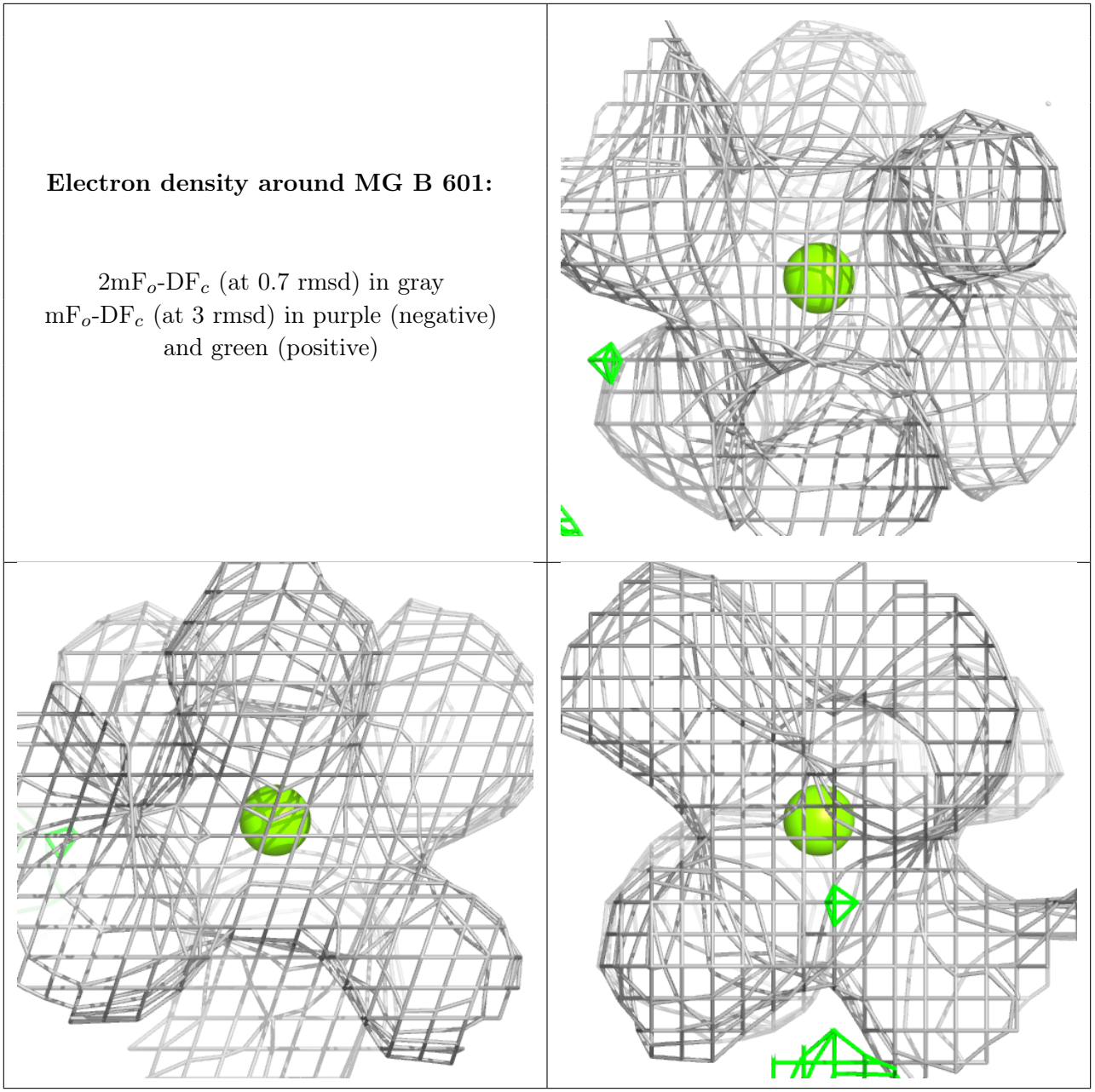
Electron density around MG A 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MG B 601:

$2mF_o$-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.