Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:51 PM UTC

PDB ID	:	9OF4 / pdb_00009of4
Title	:	Structure of the Acinetobacter baumannii Response Regulator PmrA Receiver Domain M12I Mutation
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Deposited on	:	2025-04-29
Resolution	:	2.08 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:

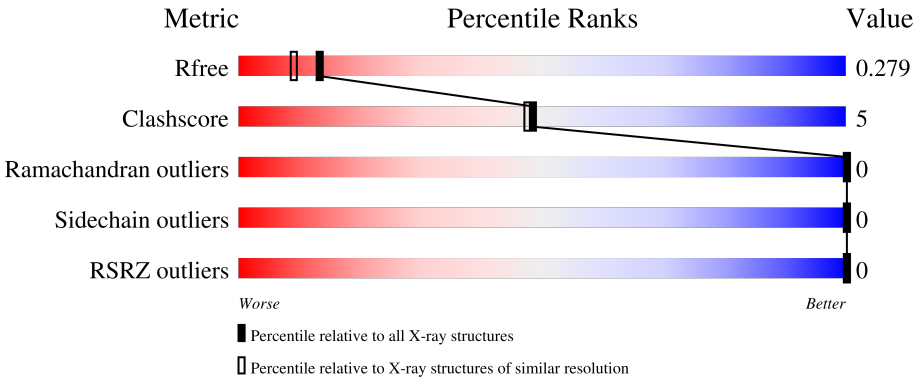
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	127	91% 6% ·
1	B	127	82% 16% ·
1	C	127	80% 17% ·
1	D	127	87% 10% ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8090 atoms, of which 4056 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 PmrA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	124	Total	C	H	N	O	S	0	0	0
			2008	633	1018	168	184	5			
1	B	124	Total	C	H	N	O	S	2	0	0
			2008	633	1018	168	184	5			
1	C	123	Total	C	H	N	O	S	0	0	0
			1991	628	1010	166	182	5			
1	D	123	Total	C	H	N	O	S	1	0	0
			1991	628	1010	166	182	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP E2FGC2
A	-1	SER	-	expression tag	UNP E2FGC2
A	0	HIS	-	expression tag	UNP E2FGC2
A	12	ILE	MET	engineered mutation	UNP E2FGC2
B	-2	GLY	-	expression tag	UNP E2FGC2
B	-1	SER	-	expression tag	UNP E2FGC2
B	0	HIS	-	expression tag	UNP E2FGC2
B	12	ILE	MET	engineered mutation	UNP E2FGC2
C	-2	GLY	-	expression tag	UNP E2FGC2
C	-1	SER	-	expression tag	UNP E2FGC2
C	0	HIS	-	expression tag	UNP E2FGC2
C	12	ILE	MET	engineered mutation	UNP E2FGC2
D	-2	GLY	-	expression tag	UNP E2FGC2
D	-1	SER	-	expression tag	UNP E2FGC2
D	0	HIS	-	expression tag	UNP E2FGC2
D	12	ILE	MET	engineered mutation	UNP E2FGC2

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is water.

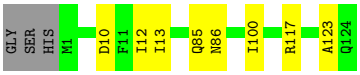
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 24 24	0	1
3	B	27	Total O 27 27	0	0
3	C	21	Total O 21 21	0	0
3	D	17	Total O 18 18	0	1

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.

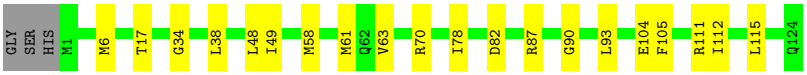
• Molecule 1: PmrA

Chain A:



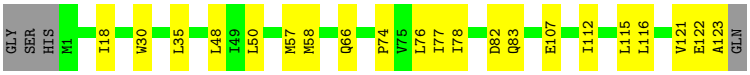
• Molecule 1: PmrA

Chain B:



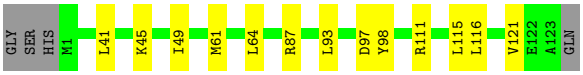
• Molecule 1: PmrA

Chain C:



• Molecule 1: PmrA

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	38.58Å 59.45Å 93.93Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	38.57 – 2.08 38.57 – 2.08	Depositor EDS
% Data completeness (in resolution range)	95.6 (38.57-2.08) 96.1 (38.57-2.08)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	5.90 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.222 , 0.279 0.223 , 0.279	Depositor DCC
R_{free} test set	1994 reflections (7.70%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 27.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.095 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8090	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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 21.56 % 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 6.8328e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.11	0/1003	0.24	0/1355
1	B	0.14	0/1003	0.29	0/1355
1	C	0.19	0/994	0.34	0/1343
1	D	0.14	0/994	0.31	0/1343
All	All	0.15	0/3994	0.30	0/5396

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	70	ARG	Sidechain

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	990	1018	1020	5	0
1	B	990	1018	1020	11	0
1	C	981	1010	1012	20	2
1	D	981	1010	1012	8	2
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	24	0	0	1	0
3	B	27	0	0	0	0
3	C	21	0	0	1	0
3	D	18	0	0	0	0
All	All	4034	4056	4064	44	2

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 5.

All (44) 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:C:48:LEU:HD12	1:C:115:LEU:HD22	1.57	0.86
1:C:74:PRO:CB	1:C:115:LEU:HD21	2.06	0.85
1:D:61:MET:HE2	1:D:93:LEU:HD13	1.70	0.72
1:C:116:LEU:HD22	1:C:121:VAL:HG21	1.78	0.65
1:D:116:LEU:HD22	1:D:121:VAL:HG21	1.79	0.65
1:D:97:ASP:OD1	1:D:98:TYR:N	2.29	0.65
1:C:74:PRO:HB3	1:C:115:LEU:HD21	1.77	0.63
1:A:100:ILE:O	3:A:202:HOH:O	2.16	0.59
1:C:115:LEU:C	1:C:115:LEU:HD23	2.30	0.56
1:A:10:ASP:OD1	1:A:13:ILE:HG22	2.07	0.56
1:C:74:PRO:HB2	1:C:115:LEU:HD21	1.89	0.55
1:D:111:ARG:O	1:D:115:LEU:HD13	2.07	0.55
1:C:77:ILE:C	1:C:78:ILE:HD12	2.32	0.53
1:C:122:GLU:O	1:C:123:ALA:HB2	2.10	0.51
1:C:35:LEU:HD13	1:C:58:MET:SD	2.52	0.50
1:D:61:MET:HA	1:D:61:MET:HE3	1.94	0.50
1:C:18:ILE:HD11	1:C:30:TRP:HB2	1.94	0.48
1:B:61:MET:HE1	1:B:90:GLY:HA2	1.95	0.48
1:C:82:ASP:O	1:C:83:GLN:OE1	2.32	0.48
1:C:35:LEU:H	1:C:35:LEU:HD22	1.79	0.47
1:C:48:LEU:HD13	1:C:112:ILE:HG23	1.97	0.47
1:B:82:ASP:O	1:B:87:ARG:NH1	2.49	0.46
1:C:78:ILE:HD12	1:C:78:ILE:N	2.31	0.45
1:C:50:LEU:HD23	1:C:76:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:MET:HE1	1:B:17:THR:HB	1.98	0.45
1:D:41:LEU:HD21	1:D:49:ILE:HD11	1.99	0.45
1:B:48:LEU:HD13	1:B:112:ILE:HG23	2.00	0.44
1:B:58:MET:HE2	1:B:63:VAL:HA	1.99	0.44
1:D:45:LYS:HD2	1:D:45:LYS:C	2.43	0.44
1:B:111:ARG:O	1:B:115:LEU:HD23	2.19	0.43
1:A:12:ILE:HD13	1:A:12:ILE:N	2.34	0.43
1:B:34:GLY:O	1:B:38:LEU:HD23	2.19	0.42
1:B:48:LEU:HD23	1:B:49:ILE:N	2.34	0.42
1:D:61:MET:HE1	1:D:64:LEU:HD23	2.01	0.42
1:C:57:MET:O	1:C:58:MET:HG2	2.20	0.42
1:B:78:ILE:HD12	1:B:78:ILE:N	2.35	0.41
1:C:66:GLN:OE1	3:C:301:HOH:O	2.22	0.41
1:C:35:LEU:CD1	1:C:58:MET:SD	3.09	0.41
1:B:104:GLU:OE2	1:B:105:PHE:N	2.54	0.41
1:A:117:ARG:HA	1:A:123:ALA:H	1.85	0.41
1:C:76:LEU:HD22	1:C:78:ILE:HD11	2.02	0.41
1:B:61:MET:HE3	1:B:93:LEU:CD1	2.51	0.41
1:C:74:PRO:CG	1:C:115:LEU:HD21	2.51	0.41
1:A:85:GLN:HG2	1:A:86:ASN:N	2.35	0.40

All (2) 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:C:107:GLU:OE2	1:D:87:ARG:NH2[2_543]	1.90	0.30
1:C:107:GLU:OE2	1:D:87:ARG:HH21[2_543]	1.43	0.17

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	122/127 (96%)	119 (98%)	3 (2%)	0	100	100
1	B	122/127 (96%)	118 (97%)	4 (3%)	0	100	100
1	C	121/127 (95%)	118 (98%)	3 (2%)	0	100	100
1	D	121/127 (95%)	119 (98%)	2 (2%)	0	100	100
All	All	486/508 (96%)	474 (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	107/109 (98%)	107 (100%)	0	100	100
1	B	107/109 (98%)	107 (100%)	0	100	100
1	C	106/109 (97%)	106 (100%)	0	100	100
1	D	106/109 (97%)	106 (100%)	0	100	100
All	All	426/436 (98%)	426 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	66	GLN
1	C	66	GLN
1	D	24	HIS
1	D	25	GLN
1	D	32	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, 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

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	124/127 (97%)	-0.92	0	100	100	21, 35, 63, 91	0
1	B	124/127 (97%)	-1.00	0	100	100	20, 30, 47, 81	0
1	C	123/127 (96%)	-1.05	0	100	100	21, 31, 54, 89	0
1	D	123/127 (96%)	-0.99	0	100	100	22, 34, 61, 97	0
All	All	494/508 (97%)	-0.99	0	100	100	20, 32, 61, 97	0

There are no RSRZ outliers to report.

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

There are no oligosaccharides in this entry.

6.4 Ligands

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.

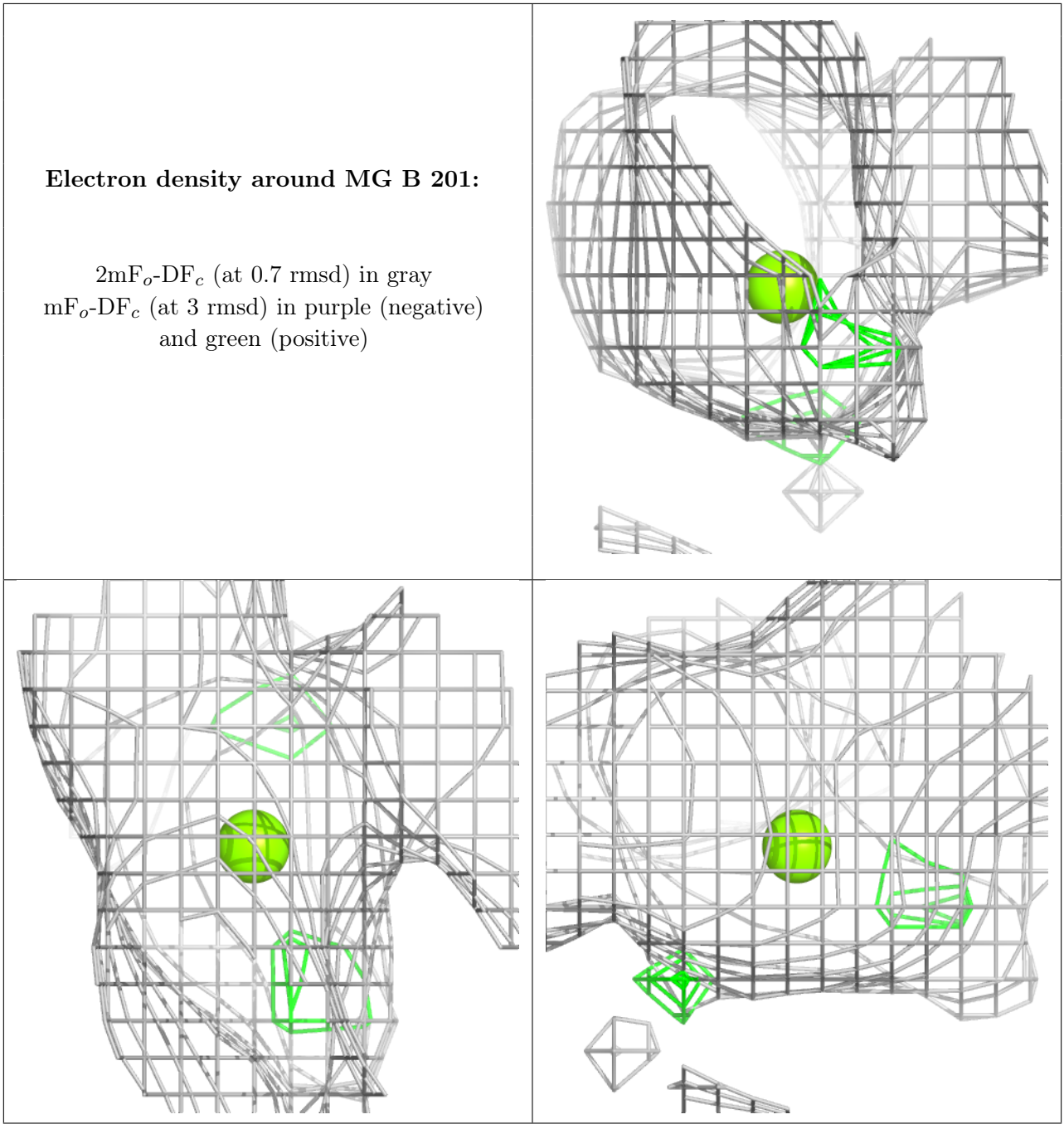
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	201	1/1	0.97	0.05	30,30,30,30	0
2	MG	C	201	1/1	0.97	0.03	30,30,30,30	0

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.

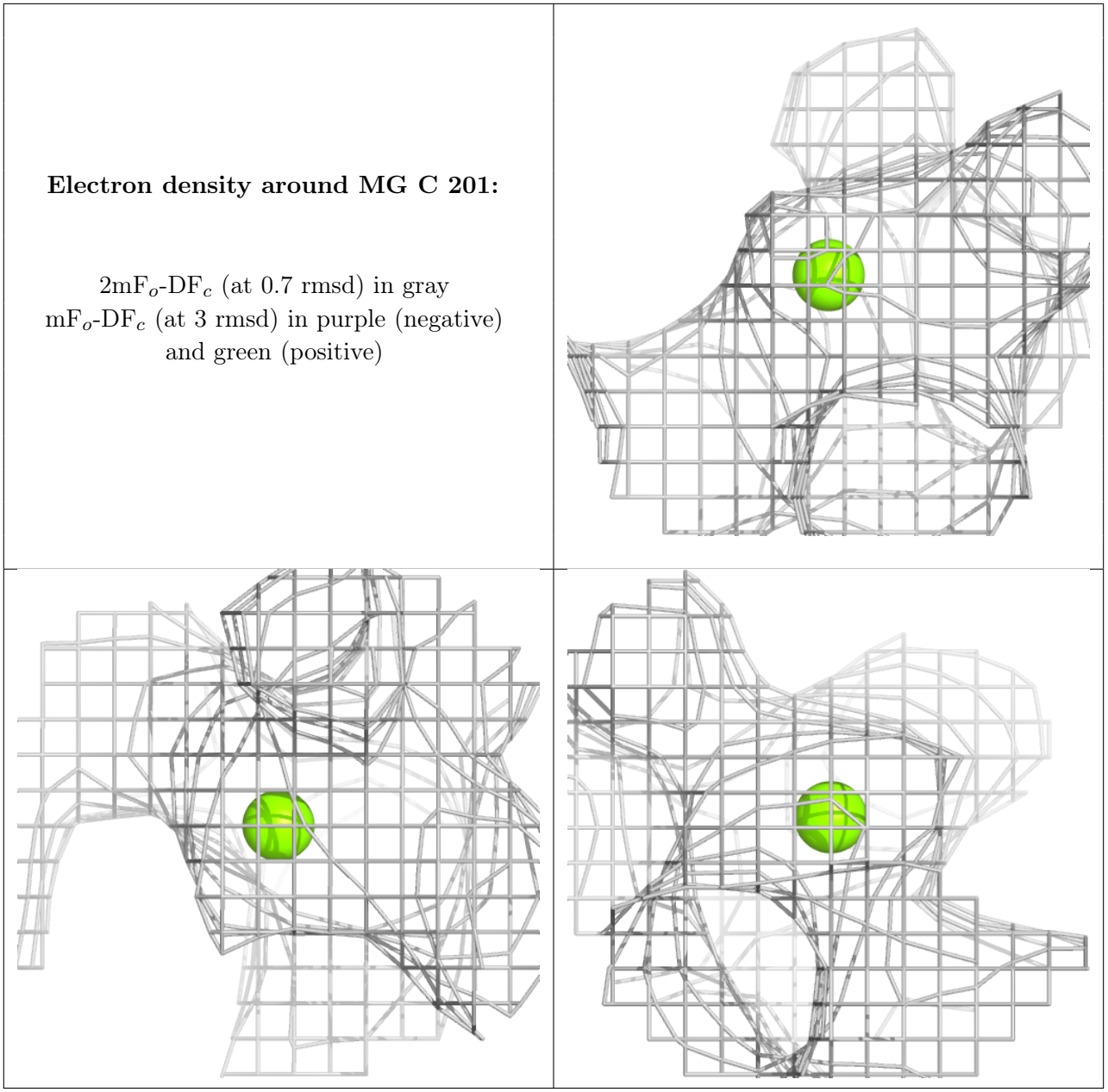
Electron density around MG B 201:

$2mF_o$-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 C 201:

$2mF_o$-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.