



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:51 PM UTC

PDB ID : 8D6J / pdb_00008d6j
Title : Human Ago2 bound to miR122(21nt) with PIWI loop swapped to AtAgo10 sequence
Authors : Xiao, Y.; MacRae, I.
Deposited on : 2022-06-06
Resolution : 2.50 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

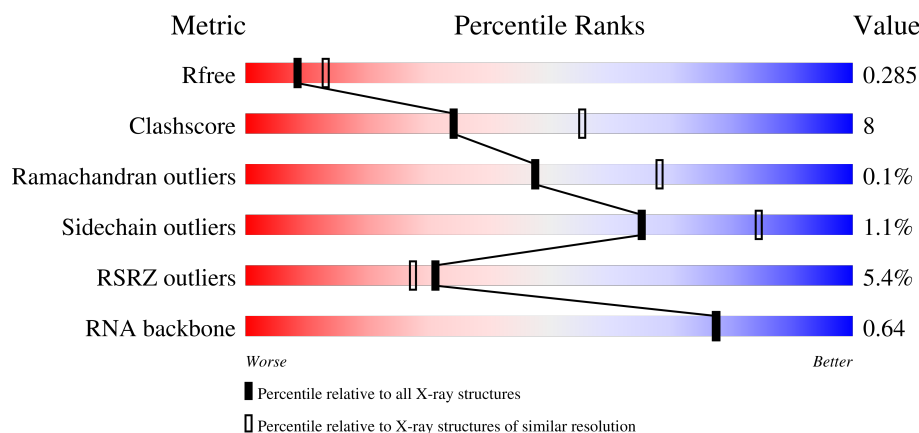
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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	859	5% 79% 14% 6%
2	B	21	48% 5% 48%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13430 atoms, of which 6656 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 Protein argonaute-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	810	Total	C	H	N	O	S	0	0	0
			13054	4131	6550	1171	1162	40			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	ASP	SER	conflict	UNP Q9UKV8
A	602	GLU	PRO	conflict	UNP Q9UKV8
A	603	ASN	ALA	conflict	UNP Q9UKV8
A	605	GLU	ASP	conflict	UNP Q9UKV8
A	606	GLU	GLY	conflict	UNP Q9UKV8
A	607	SER	LYS	conflict	UNP Q9UKV8
A	608	SER	LYS	conflict	UNP Q9UKV8
A	824	ALA	SER	conflict	UNP Q9UKV8
A	828	ASP	SER	conflict	UNP Q9UKV8
A	831	ASP	SER	conflict	UNP Q9UKV8
A	834	ALA	SER	conflict	UNP Q9UKV8

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*GP*GP*AP*GP*UP*GP*UP*GP*AP*CP*AP*AP*UP*GP*GP*UP*GP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	11	Total	C	H	N	O	P	0	0	0
			325	95	106	35	78	11			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total 49	O 49	0	0
4	B	1	Total 1	O 1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.30Å 107.51Å 68.71Å 90.00° 106.90° 90.00°	Depositor
Resolution (Å)	39.22 – 2.50 39.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (39.22-2.50) 93.4 (39.22-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.57 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.232 , 0.284 0.232 , 0.285	Depositor DCC
R_{free} test set	2030 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13430	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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

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	0.17	0/6653	0.30	0/9000
2	B	0.10	0/242	0.26	0/372
All	All	0.17	0/6895	0.30	0/9372

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	6504	6550	6550	102	1
2	B	219	106	106	1	0
3	A	1	0	0	0	0
4	A	49	0	0	12	0
4	B	1	0	0	0	0
All	All	6774	6656	6656	102	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 8.

All (102) 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:150:ARG:HG3	1:A:151:LEU:N	1.96	0.79
1:A:473:GLN:O	4:A:1001:HOH:O	2.00	0.79
1:A:521:ILE:HD11	1:A:552:VAL:HG21	1.66	0.78
1:A:78:MET:HE1	1:A:130:VAL:HG11	1.69	0.75
1:A:539:VAL:HG23	1:A:540:LEU:HD12	1.70	0.73
1:A:51:LYS:O	1:A:52:ILE:HG23	1.87	0.73
1:A:477:ILE:N	4:A:1001:HOH:O	2.02	0.72
1:A:72:ARG:NH1	1:A:94:PHE:O	2.24	0.71
1:A:507:HIS:O	1:A:511:THR:OG1	2.01	0.71
1:A:641:ASP:OD2	4:A:1002:HOH:O	2.09	0.70
1:A:521:ILE:CD1	1:A:552:VAL:HG21	2.22	0.70
1:A:51:LYS:O	1:A:51:LYS:HD2	1.92	0.69
1:A:729:ASN:OD1	4:A:1003:HOH:O	2.12	0.68
1:A:478:SER:OG	1:A:485:ILE:HG22	1.94	0.67
1:A:517:LEU:HD21	1:A:519:VAL:HG23	1.76	0.67
1:A:90:ARG:NH1	1:A:104:MET:HE2	2.12	0.65
1:A:502:GLU:OE2	1:A:506:ARG:NE	2.29	0.65
1:A:34:SER:OG	4:A:1004:HOH:O	2.14	0.65
1:A:150:ARG:HG3	1:A:151:LEU:H	1.61	0.64
1:A:82:PHE:CE2	1:A:115:LEU:HD13	2.33	0.63
1:A:210:LEU:HB2	4:A:1026:HOH:O	1.99	0.62
1:A:413:LEU:O	4:A:1005:HOH:O	2.15	0.62
1:A:491:PHE:CD2	1:A:508:LEU:HD21	2.34	0.62
1:A:468:LYS:O	1:A:472:GLU:HG3	2.00	0.61
1:A:184:ALA:O	1:A:186:GLU:N	2.34	0.60
1:A:222:THR:HG23	1:A:224:PHE:CE2	2.36	0.60
1:A:61:ILE:HG12	1:A:130:VAL:HG22	1.83	0.60
1:A:502:GLU:OE2	1:A:506:ARG:NH2	2.36	0.59
1:A:90:ARG:HD2	1:A:104:MET:CE	2.32	0.58
1:A:230:VAL:O	1:A:234:VAL:HG23	2.04	0.57
1:A:97:ARG:C	1:A:98:LYS:HD2	2.31	0.56
1:A:425:LYS:O	1:A:425:LYS:HD2	2.05	0.55
1:A:470:PHE:CD1	1:A:552:VAL:HG22	2.42	0.55
1:A:438:ARG:N	1:A:438:ARG:HD3	2.22	0.54
1:A:134:TRP:NE1	1:A:136:SER:O	2.40	0.54
1:A:474:LEU:C	4:A:1001:HOH:O	2.52	0.52
1:A:61:ILE:CG1	1:A:130:VAL:HG22	2.40	0.52
1:A:169:LEU:HB3	1:A:170:PRO:HD3	1.90	0.52
1:A:51:LYS:O	1:A:52:ILE:CG2	2.56	0.52
1:A:609:PRO:O	1:A:814:ARG:NH2	2.42	0.51
1:A:402:LYS:HD3	4:A:1024:HOH:O	2.10	0.51
1:A:488:GLN:HB3	1:A:489:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:PHE:HD2	1:A:508:LEU:HD21	1.75	0.51
1:A:853:LEU:C	1:A:853:LEU:HD23	2.35	0.51
1:A:475:ARG:NH1	1:A:488:GLN:OE1	2.44	0.50
1:A:136:SER:OG	1:A:137:CYS:N	2.44	0.50
1:A:729:ASN:HA	4:A:1003:HOH:O	2.10	0.50
1:A:182:PHE:CZ	1:A:222:THR:HG22	2.47	0.50
1:A:638:ILE:HD12	1:A:679:VAL:HG22	1.94	0.50
1:A:556:THR:CG2	1:A:558:GLN:HE21	2.25	0.49
1:A:603:ASN:HD22	1:A:603:ASN:C	2.20	0.49
1:A:90:ARG:HD2	1:A:104:MET:HE2	1.95	0.49
1:A:599:THR:HG22	1:A:810:ALA:HB1	1.94	0.48
1:A:250:LEU:HD12	1:A:326:PRO:HD3	1.95	0.48
1:A:448:ILE:HG23	1:A:485:ILE:HA	1.95	0.48
1:A:502:GLU:HB3	1:A:503:PRO:HD3	1.96	0.47
1:A:853:LEU:HD23	1:A:853:LEU:O	2.14	0.47
1:A:455:CYS:HA	1:A:521:ILE:HB	1.97	0.47
1:A:78:MET:CE	1:A:130:VAL:HG11	2.41	0.47
1:A:797:VAL:HG23	1:A:799:ILE:O	2.15	0.46
1:A:475:ARG:HG2	1:A:485:ILE:HG23	1.98	0.45
1:A:502:GLU:OE2	1:A:506:ARG:CZ	2.64	0.45
1:A:459:GLN:N	1:A:460:ARG:NH1	2.65	0.45
1:A:69:ARG:NH2	1:A:72:ARG:HE	2.15	0.45
1:A:269:ILE:HD11	1:A:339:LEU:HD13	1.98	0.44
1:A:505:PHE:HE1	1:A:518:VAL:HG11	1.81	0.44
1:A:502:GLU:CD	1:A:506:ARG:HE	2.24	0.44
1:A:212:LYS:HG3	1:A:214:MET:HE2	1.98	0.44
1:A:248:LYS:N	1:A:248:LYS:HD3	2.33	0.44
1:A:51:LYS:HD2	1:A:51:LYS:C	2.42	0.44
1:A:680:LEU:HD11	1:A:684:LEU:HD22	2.00	0.44
1:A:483:MET:HE1	1:A:567:ILE:HD11	1.99	0.43
1:A:670:GLY:N	1:A:707:VAL:O	2.51	0.43
1:A:151:LEU:O	1:A:153:SER:N	2.51	0.43
1:A:566:LYS:NZ	1:A:859:ALA:OXT	2.51	0.43
1:A:425:LYS:O	1:A:425:LYS:CD	2.67	0.43
1:A:90:ARG:HD2	1:A:104:MET:HE3	2.00	0.43
1:A:96:GLY:O	1:A:97:ARG:C	2.60	0.43
1:A:470:PHE:CE1	1:A:552:VAL:HG22	2.54	0.42
1:A:558:GLN:H	1:A:558:GLN:CD	2.28	0.42
1:A:55:TYR:CZ	1:A:105:PRO:HG3	2.55	0.42
1:A:446:ILE:HD13	1:A:571:LEU:HB3	2.02	0.42
1:A:372:ALA:HB3	1:A:373:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:THR:HG23	1:A:254:GLN:H	1.85	0.41
1:A:426:ALA:N	4:A:1008:HOH:O	2.36	0.41
1:A:425:LYS:O	1:A:426:ALA:C	2.63	0.41
1:A:423:ARG:NE	1:A:441:GLN:OE1	2.54	0.41
1:A:483:MET:HG3	1:A:568:ASN:OD1	2.21	0.41
1:A:282:CYS:SG	1:A:329:GLN:HG2	2.61	0.41
1:A:551:ASN:ND2	2:B:2:G:OP2	2.53	0.41
1:A:483:MET:HE2	1:A:483:MET:HB3	1.94	0.41
1:A:210:LEU:HG	1:A:211:TRP:CE3	2.56	0.41
1:A:459:GLN:O	1:A:463:THR:N	2.53	0.41
1:A:556:THR:CG2	1:A:558:GLN:NE2	2.84	0.41
1:A:357:THR:O	1:A:361:THR:HG23	2.21	0.41
1:A:737:ASP:HA	1:A:741:THR:HG21	2.03	0.41
1:A:485:ILE:HG23	1:A:485:ILE:O	2.20	0.40
1:A:769:TRP:NE1	1:A:771:ASP:OD1	2.49	0.40
1:A:451:TRP:CE2	1:A:485:ILE:HD11	2.57	0.40
1:A:69:ARG:NH1	1:A:171:SER:O	2.54	0.40
1:A:425:LYS:HD2	1:A:425:LYS:C	2.47	0.40
1:A:476:LYS:N	4:A:1001:HOH:O	2.55	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:287:ARG:HH22	1:A:398:GLY:O[1_554]	1.56	0.04

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	798/859 (93%)	749 (94%)	48 (6%)	1 (0%)	48 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	SER

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	720/752 (96%)	712 (99%)	8 (1%)	65 84

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	GLU
1	A	115	LEU
1	A	118	THR
1	A	207	ARG
1	A	212	LYS
1	A	448	ILE
1	A	603	ASN
1	A	608	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	A	291	HIS
1	A	336	HIS
1	A	439	ASN
1	A	486	GLN
1	A	548	GLN
1	A	558	GLN
1	A	603	ASN
1	A	623	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	8/21 (38%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 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 ⓘ

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, 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	810/859 (94%)	0.56	44 (5%) 31 27	31, 64, 95, 113	0
2	B	11/21 (52%)	0.01	0 100 100	40, 56, 75, 91	0
All	All	821/880 (93%)	0.56	44 (5%) 31 27	31, 64, 95, 113	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	PHE	3.5
1	A	151	LEU	3.5
1	A	552	VAL	3.5
1	A	674	GLY	3.1
1	A	109	GLY	3.1
1	A	818	VAL	3.0
1	A	137	CYS	2.9
1	A	120	PRO	2.9
1	A	132	ILE	2.8
1	A	125	ASP	2.8
1	A	117	VAL	2.7
1	A	482	GLY	2.7
1	A	127	ILE	2.7
1	A	113	VAL	2.7
1	A	96	GLY	2.6
1	A	304	VAL	2.6
1	A	59	LEU	2.6
1	A	491	PHE	2.5
1	A	136	SER	2.5
1	A	146	ALA	2.5
1	A	188	CYS	2.5
1	A	54	ILE	2.5
1	A	130	VAL	2.5
1	A	465	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	61	ILE	2.4
1	A	495	ALA	2.4
1	A	817	LEU	2.4
1	A	156	PHE	2.3
1	A	53	ASP	2.3
1	A	86	ILE	2.2
1	A	250	LEU	2.2
1	A	270	THR	2.2
1	A	604	GLY	2.2
1	A	481	ALA	2.2
1	A	52	ILE	2.2
1	A	837	ARG	2.1
1	A	469	SER	2.1
1	A	104	MET	2.1
1	A	79	VAL	2.1
1	A	467	LEU	2.1
1	A	135	VAL	2.0
1	A	90	ARG	2.0
1	A	119	LEU	2.0
1	A	756	ILE	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.

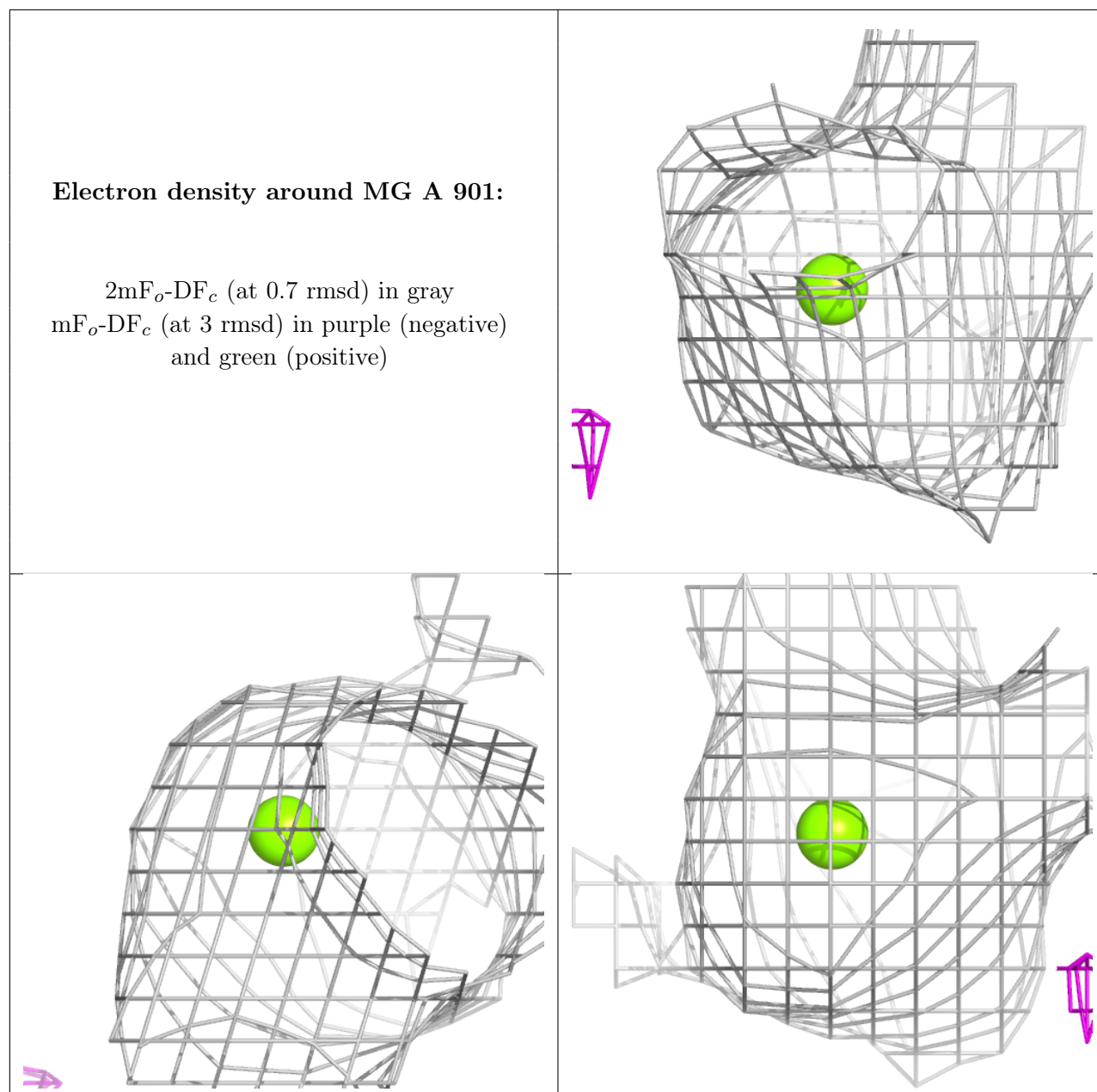
6.4 Ligands [i](#)

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	MG	A	901	1/1	0.95	0.12	50,50,50,50	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.