



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 21, 2025 – 06:07 PM EDT

PDB ID : 9CKH / pdb_00009ckh
Title : [d2d3-2Ag] Tensegrity triangle with deazapurines on the helical and center strands with two deazaA:Ag+:T base pairs
Authors : Vecchioni, S.; Jong, M.A.; Woloszyn, K.; Sha, R.; Ohayon, Y.P.; Gallindo, M.A.; Lopez Chamorro, C.
Deposited on : 2024-07-08
Resolution : 5.92 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.44

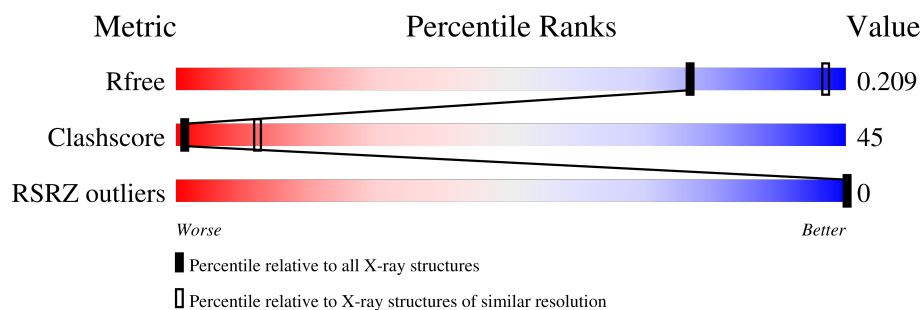
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.92 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	1076 (7.82-4.00)
Clashscore	180529	1116 (7.82-4.00)
RSRZ outliers	164620	1071 (7.82-4.00)

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	21	
2	B	7	
3	C	6	
4	D	8	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 857 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 DNA chain called DNA (5'-D(*GP*AP*(7GU)P*CP*(7DA)P*(7GU)P*CP*CP*TP*(7GU)P*TP*(7DA)P*CP*(7GU)P*(7GU)P*(7DA)P*CP*(7DA)P*TP*CP*(7DA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	P	0	0	0
			429	214	74	121	20			

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*CP*(7GU)P*TP*(7DA)P*CP*(7DA))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	P	0	0	0
			141	70	23	41	7			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*CP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	P	0	0	0
			124	58	23	37	6			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*CP*TP*GP*AP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	8	Total	C	N	O	P	0	0	0
			161	79	26	49	7			


- Molecule 5 is SILVER ION (CCD ID: AG) (formula: Ag) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ag	0	0
			1	1		
5	D	1	Total	Ag	0	0
			1	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: DNA (5'-D(*GP*AP*(7GU)P*CP*(7DA)P*(7GU)P*CP*CP*TP*(7GU)P*TP*(7DA)P*CP*(7GU)P*(7GU)P*(7DA)P*CP*(7DA)P*TP*CP*(7DA))-3')

Chain A: 



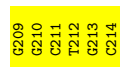
- Molecule 2: DNA (5'-D(P*CP*CP*(7GU)P*TP*(7DA)P*CP*(7DA))-3')

Chain B: 



- Molecule 3: DNA (5'-D(P*GP*GP*CP*TP*GP*C)-3')

Chain C: 



- Molecule 4: DNA (5'-D(*TP*CP*TP*GP*AP*TP*GP*T)-3')

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	123.28Å 123.28Å 62.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.67 – 5.92 19.67 – 5.92	Depositor EDS
% Data completeness (in resolution range)	79.0 (19.67-5.92) 77.7 (19.67-5.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 5.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.161 , 0.179 0.200 , 0.209	Depositor DCC
R_{free} test set	72 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	247.0	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.108 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	857	wwPDB-VP
Average B, all atoms (Å ²)	260.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: 7DA, AG, 7GU

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	0.45	0/231	0.69	0/338
2	B	0.35	0/82	0.54	0/118
3	C	0.30	0/138	0.48	0/211
4	D	0.36	0/179	0.60	0/275
All	All	0.38	0/630	0.61	0/942

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	429	0	245	32	0
2	B	141	0	82	10	0
3	C	124	0	68	11	0
4	D	161	0	93	11	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
All	All	857	0	488	55	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 45.

The worst 5 of 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:A:120:DC:O2	4:D:204:DG:N2	1.71	1.22
1:A:120:DC:N3	4:D:204:DG:N1	2.08	0.99
1:A:102:DA:H2'	1:A:103:7GU:H8	1.45	0.95
1:A:102:DA:H2'	1:A:103:7GU:C8	2.01	0.90
1:A:107:DC:O2	3:C:210:DG:N2	2.10	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

13 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	7DA	A	121	1,4	18,23,24	3.73	9 (50%)	18,33,36	4.02	7 (38%)
1	7GU	A	110	1,2	20,24,25	3.79	12 (60%)	21,35,38	5.00	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	7DA	A	112	1,2	18,23,24	3.75	10 (55%)	18,33,36	4.30	10 (55%)
1	7GU	A	114	1,2	20,24,25	3.82	13 (65%)	21,35,38	5.00	5 (23%)
1	7GU	A	115	1,2	20,24,25	3.82	12 (60%)	21,35,38	5.37	7 (33%)
2	7GU	B	121	1,2	20,24,25	3.76	14 (70%)	21,35,38	5.07	5 (23%)
1	7GU	A	103	1,3	20,24,25	3.68	12 (60%)	21,35,38	4.99	6 (28%)
2	7DA	B	125	1,2	18,23,24	3.84	9 (50%)	18,33,36	4.32	5 (27%)
1	7DA	A	118	1,4	18,23,24	3.95	10 (55%)	18,33,36	3.97	6 (33%)
1	7DA	A	116	1,5	18,23,24	3.69	10 (55%)	18,33,36	4.30	6 (33%)
1	7DA	A	105	1,3	18,23,24	3.90	10 (55%)	18,33,36	3.55	4 (22%)
1	7GU	A	106	1,3	20,24,25	3.81	12 (60%)	21,35,38	4.75	5 (23%)
2	7DA	B	123	5,2	18,23,24	3.72	9 (50%)	18,33,36	4.54	6 (33%)

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
1	7DA	A	121	1,4	-	3/3/21/22	0/3/3/3
1	7GU	A	110	1,2	-	2/3/21/22	0/3/3/3
1	7DA	A	112	1,2	-	2/3/21/22	0/3/3/3
1	7GU	A	114	1,2	-	0/3/21/22	0/3/3/3
1	7GU	A	115	1,2	-	2/3/21/22	0/3/3/3
2	7GU	B	121	1,2	-	2/3/21/22	0/3/3/3
1	7GU	A	103	1,3	-	2/3/21/22	0/3/3/3
2	7DA	B	125	1,2	-	1/3/21/22	0/3/3/3
1	7DA	A	118	1,4	-	2/3/21/22	0/3/3/3
1	7DA	A	116	1,5	-	1/3/21/22	0/3/3/3
1	7DA	A	105	1,3	-	2/3/21/22	0/3/3/3
1	7GU	A	106	1,3	-	0/3/21/22	0/3/3/3
2	7DA	B	123	5,2	-	2/3/21/22	0/3/3/3

The worst 5 of 142 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	121	7GU	C2'-C3'	-8.04	1.32	1.52
1	A	115	7GU	C2'-C3'	-7.97	1.32	1.52
1	A	118	7DA	C6-C5	-7.91	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	7DA	C6-C5	-7.85	1.37	1.45
1	A	114	7GU	C2'-C3'	-7.75	1.33	1.52

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	7GU	C8-N9-C1'	23.41	148.49	125.37
2	B	121	7GU	C8-N9-C1'	22.06	147.16	125.37
1	A	114	7GU	C8-N9-C1'	21.91	147.01	125.37
1	A	103	7GU	C8-N9-C1'	21.75	146.86	125.37
1	A	110	7GU	C8-N9-C1'	21.68	146.78	125.37

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	103	7GU	C3'-C4'-C5'-O5'
1	A	105	7DA	O4'-C4'-C5'-O5'
1	A	121	7DA	O4'-C4'-C5'-O5'
1	A	103	7GU	O4'-C4'-C5'-O5'
1	A	110	7GU	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	121	7DA	3	0
1	A	110	7GU	2	0
1	A	112	7DA	2	0
1	A	114	7GU	2	0
1	A	115	7GU	1	0
2	B	121	7GU	2	0
1	A	103	7GU	5	0
2	B	125	7DA	1	0
1	A	118	7DA	1	0
1	A	116	7DA	1	0
1	A	105	7DA	1	0
2	B	123	7DA	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	11/21 (52%)	-0.19	0 100 100	222, 242, 298, 299	0
2	B	4/7 (57%)	0.35	0 100 100	195, 232, 246, 257	0
3	C	6/6 (100%)	-0.22	0 100 100	219, 243, 328, 334	0
4	D	8/8 (100%)	0.08	0 100 100	242, 253, 331, 335	0
All	All	29/42 (69%)	-0.05	0 100 100	195, 248, 331, 335	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	7GU	A	106	22/23	0.81	0.10	280,331,350,359	0
2	7DA	B	123	21/22	0.83	0.09	207,222,284,296	0
1	7DA	A	116	21/22	0.84	0.16	225,237,243,248	0
1	7DA	A	105	21/22	0.88	0.07	272,306,331,346	0
1	7GU	A	103	22/23	0.88	0.05	251,280,297,303	0
1	7GU	A	110	22/23	0.90	0.09	217,234,299,316	0
1	7DA	A	121	21/22	0.91	0.10	221,263,277,282	0
1	7GU	A	115	22/23	0.93	0.11	214,223,244,286	0
2	7GU	B	121	22/23	0.93	0.09	224,234,254,261	0
1	7DA	A	112	21/22	0.93	0.10	204,234,253,261	0
1	7DA	A	118	21/22	0.95	0.09	228,235,241,260	0
1	7GU	A	114	22/23	0.95	0.10	210,223,230,240	0
2	7DA	B	125	21/22	0.96	0.15	201,220,227,229	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

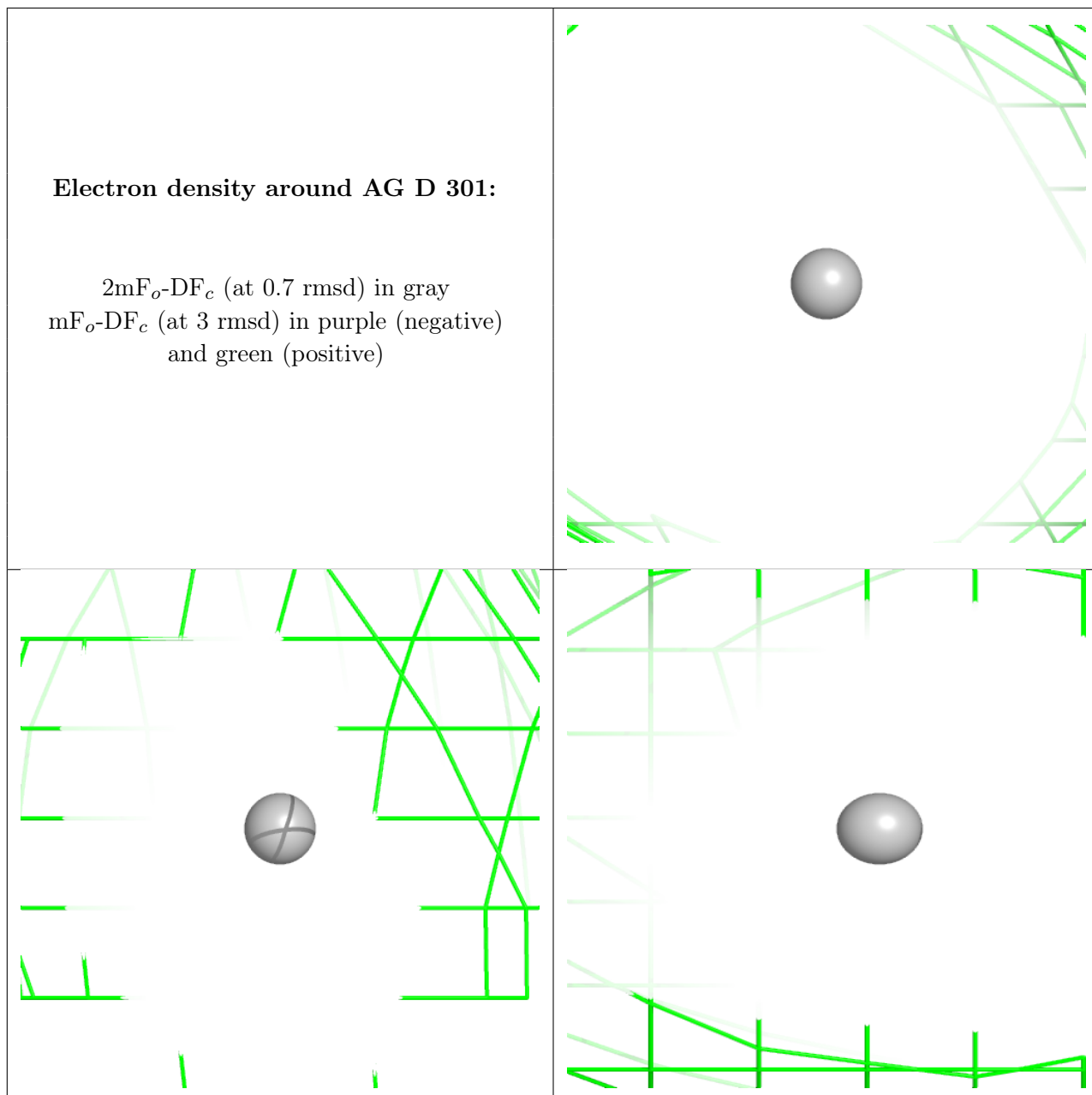
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

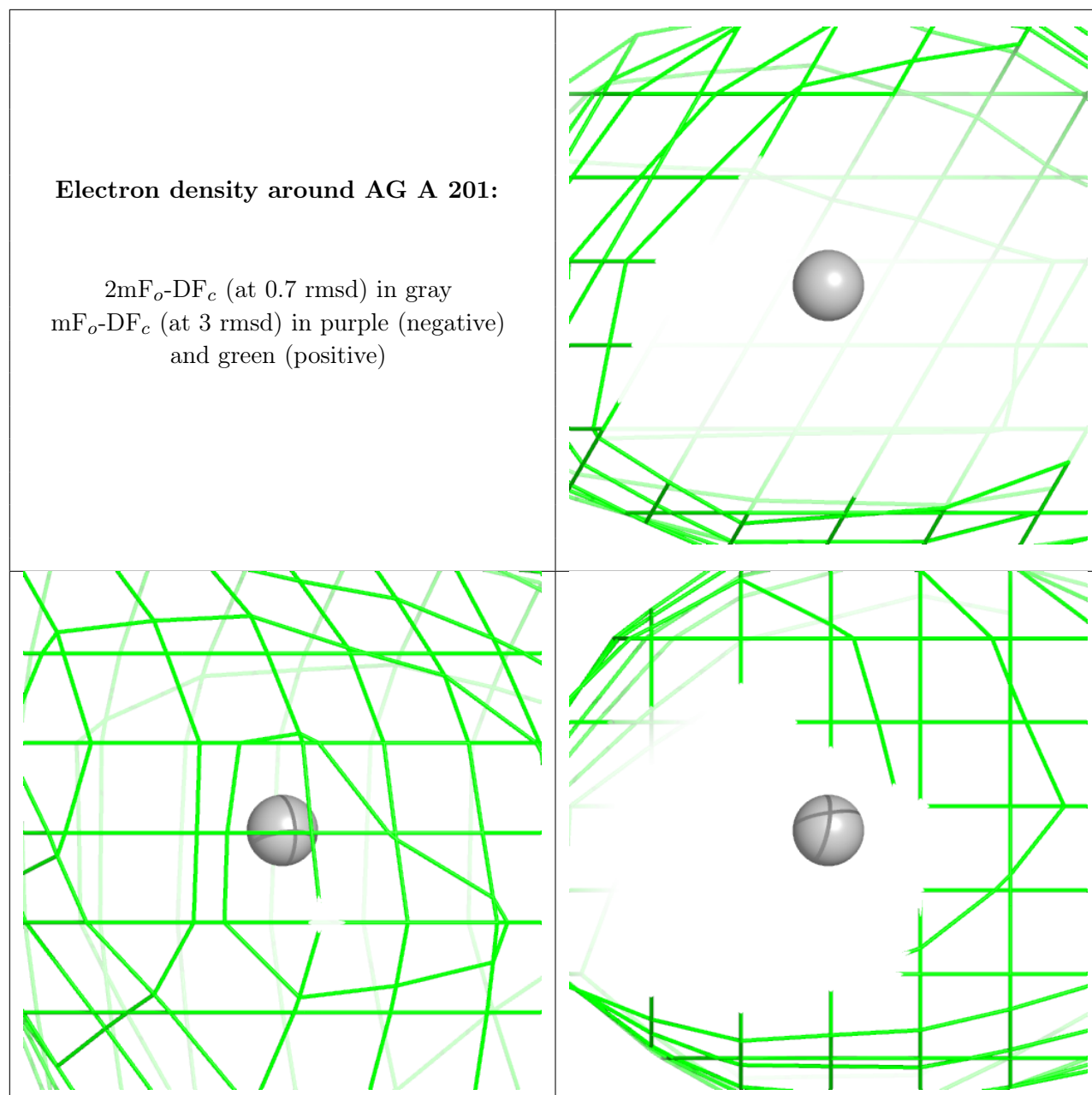
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	AG	D	301	1/1	0.95	0.27	240,240,240,240	0
5	AG	A	201	1/1	0.98	0.14	230,230,230,230	0

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 AG D 301:

$2mF_o-DF_c$ (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.