



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 20, 2026 – 10:20 am BST

PDB ID : 9T4Y / pdb_00009t4y
Title : apo form of XN-IL lectin from Xenorhabdus nematophila
Authors : Korsak, M.; Wimmerova, M.
Deposited on : 2025-11-03
Resolution : 1.56 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 Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
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

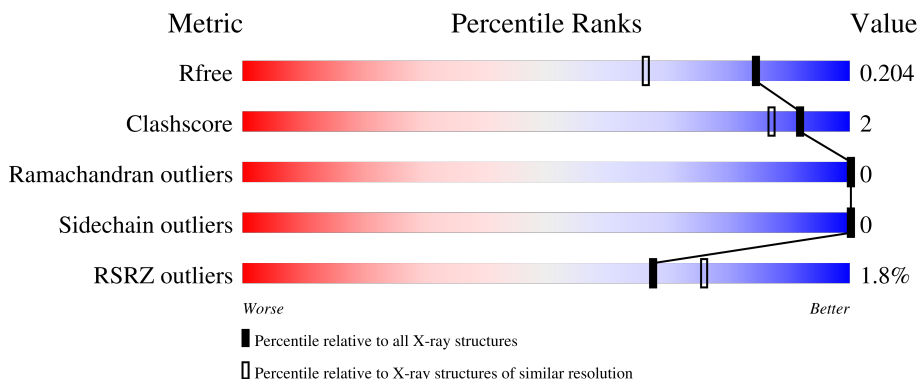
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	AAA	125	 97%
1	BBB	125	 99%
1	CCC	125	 94% 5%
1	DDD	125	 98%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PEG	BBB	204	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4460 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 PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	AAA	125	Total	C	N	O	0	0	0	
			959	623	152	184				
1	BBB	124	Total	C	N	O	S	0	1	0
			961	621	155	184	1			
1	CCC	124	Total	C	N	O	0	2	0	
			950	616	152	182				
1	DDD	124	Total	C	N	O	0	0	0	
			941	609	152	180				

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	11	LYS	ARG	conflict	UNP D3VE08
BBB	11	LYS	ARG	conflict	UNP D3VE08
CCC	11	LYS	ARG	conflict	UNP D3VE08
DDD	11	LYS	ARG	conflict	UNP D3VE08

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AAA	1	Total	Ca	0	0
			1	1		
2	BBB	1	Total	Ca	0	0
			1	1		
2	CCC	1	Total	Ca	0	0
			1	1		
2	DDD	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total O S 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	0
3	AAA	1	Total O S 5 4 1	0	0
3	CCC	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

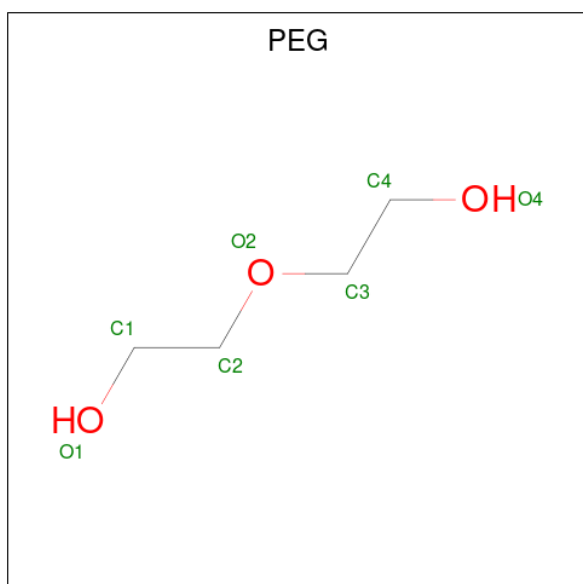
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total Mg 1 1	0	0
4	BBB	1	Total Mg 1 1	0	0
4	CCC	1	Total Mg 1 1	0	0
4	DDD	1	Total Mg 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total C O 4 2 2	0	0
5	CCC	1	Total C O 4 2 2	0	0
5	CCC	1	Total C O 4 2 2	0	0
5	DDD	1	Total C O 4 2 2	0	0
5	DDD	1	Total C O 4 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	BBB	1	Total C O 7 4 3	0	0
6	CCC	1	Total C O 7 4 3	0	0
6	CCC	1	Total C O 7 4 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	148	Total O 148 148	0	0
7	BBB	148	Total O 148 148	0	0
7	CCC	150	Total O 150 150	0	0
7	DDD	134	Total O 134 134	0	0

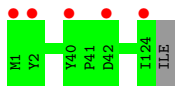
3 Residue-property plots [i](#)

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.

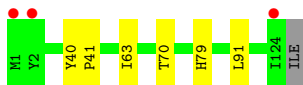
- Molecule 1: PA-I galactophilic lectin (PA-IL) (Galactose-binding lectin)



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.83Å 76.69Å 148.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 1.56 48.14 – 1.56	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.14-1.56) 99.9 (48.14-1.56)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.56Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.171 , 0.197 0.183 , 0.204	Depositor DCC
R_{free} test set	4396 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4460	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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, CA, SO4, PEG, EDO

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	AAA	0.96	0/985	1.11	0/1344
1	BBB	0.95	0/987	1.06	0/1344
1	CCC	1.02	0/976	1.05	0/1334
1	DDD	1.01	0/967	1.09	0/1321
All	All	0.99	0/3915	1.08	0/5343

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	AAA	959	0	936	2	0
1	BBB	961	0	943	0	0
1	CCC	950	0	908	4	0
1	DDD	941	0	909	1	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
3	AAA	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CCC	5	0	0	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	CCC	1	0	0	0	0
4	DDD	1	0	0	0	0
5	BBB	4	0	6	0	0
5	CCC	8	0	12	0	0
5	DDD	8	0	12	0	0
6	BBB	7	0	9	4	0
6	CCC	14	0	20	2	0
7	AAA	148	0	0	1	0
7	BBB	148	0	0	1	0
7	CCC	150	0	0	1	0
7	DDD	134	0	0	0	0
All	All	4460	0	3755	12	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 2.

The worst 5 of 12 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)
6:BBB:204:PEG:H31	6:BBB:204:PEG:O1	1.67	0.92
6:BBB:204:PEG:O1	6:BBB:204:PEG:C3	2.18	0.91
6:BBB:204:PEG:H22	7:BBB:423:HOH:O	1.90	0.70
1:CCC:63:ILE:HD11	1:CCC:91:LEU:HD23	1.77	0.65
1:AAA:45:TRP:HB2	1:AAA:52:LEU:HD22	1.95	0.49

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	AAA	123/125 (98%)	122 (99%)	1 (1%)	0	100	100
1	BBB	123/125 (98%)	123 (100%)	0	0	100	100
1	CCC	124/125 (99%)	122 (98%)	2 (2%)	0	100	100
1	DDD	122/125 (98%)	122 (100%)	0	0	100	100
All	All	492/500 (98%)	489 (99%)	3 (1%)	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	AAA	100/104 (96%)	100 (100%)	0	100	100
1	BBB	102/104 (98%)	102 (100%)	0	100	100
1	CCC	96/104 (92%)	96 (100%)	0	100	100
1	DDD	97/104 (93%)	97 (100%)	0	100	100
All	All	395/416 (95%)	395 (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. There are no such sidechains identified.

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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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
5	EDO	CCC	206	-	3,3,3	0.25	0	2,2,2	0.14	0
6	PEG	BBB	204	-	6,6,6	0.72	0	5,5,5	0.48	0
6	PEG	CCC	205	-	6,6,6	0.25	0	5,5,5	0.32	0
5	EDO	BBB	203	-	3,3,3	0.10	0	2,2,2	0.23	0
5	EDO	CCC	204	-	3,3,3	0.09	0	2,2,2	0.33	0
5	EDO	DDD	204	-	3,3,3	0.28	0	2,2,2	0.38	0
5	EDO	DDD	203	-	3,3,3	0.29	0	2,2,2	0.37	0
3	SO4	CCC	202	-	4,4,4	0.18	0	6,6,6	0.30	0
3	SO4	AAA	203	-	4,4,4	0.38	0	6,6,6	0.14	0
3	SO4	AAA	202	-	4,4,4	0.10	0	6,6,6	0.14	0
6	PEG	CCC	207	-	6,6,6	0.28	0	5,5,5	0.53	0
3	SO4	AAA	204	-	4,4,4	0.34	0	6,6,6	0.10	0

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
5	EDO	CCC	206	-	-	1/1/1/1	-
6	PEG	CCC	205	-	-	3/4/4/4	-
5	EDO	BBB	203	-	-	0/1/1/1	-
5	EDO	CCC	204	-	-	1/1/1/1	-
5	EDO	DDD	204	-	-	1/1/1/1	-
5	EDO	DDD	203	-	-	0/1/1/1	-
6	PEG	CCC	207	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	BBB	204	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	CCC	206	EDO	O1-C1-C2-O2
5	DDD	204	EDO	O1-C1-C2-O2
6	BBB	204	PEG	C1-C2-O2-C3
5	CCC	204	EDO	O1-C1-C2-O2
6	CCC	205	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	BBB	204	PEG	4	0
6	CCC	205	PEG	1	0
6	CCC	207	PEG	1	0

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	AAA	125/125 (100%)	0.05	1 (0%) 82 87	9, 15, 26, 36	0
1	BBB	124/125 (99%)	-0.13	5 (4%) 42 50	7, 13, 23, 38	1 (0%)
1	CCC	124/125 (99%)	-0.18	3 (2%) 59 67	7, 13, 22, 33	2 (1%)
1	DDD	124/125 (99%)	-0.08	0 100 100	9, 15, 24, 32	0
All	All	497/500 (99%)	-0.08	9 (1%) 67 76	7, 14, 25, 38	3 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	124	ILE	4.5
1	AAA	125	ILE	3.7
1	BBB	1	MET	3.5
1	CCC	124	ILE	2.7
1	CCC	1	MET	2.6

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](#)

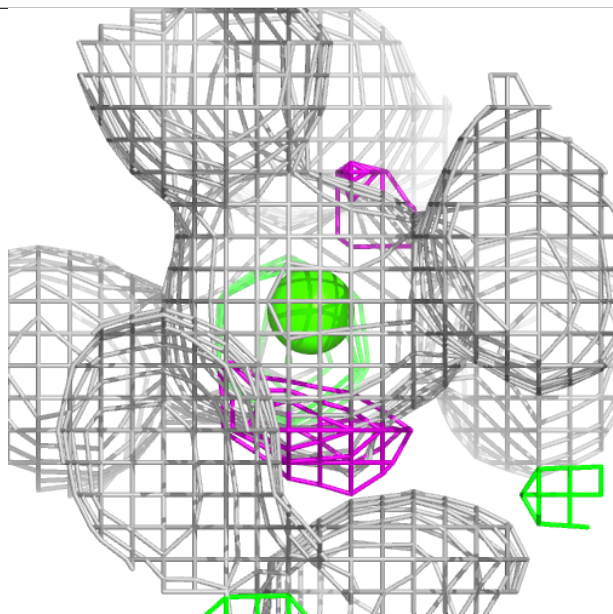
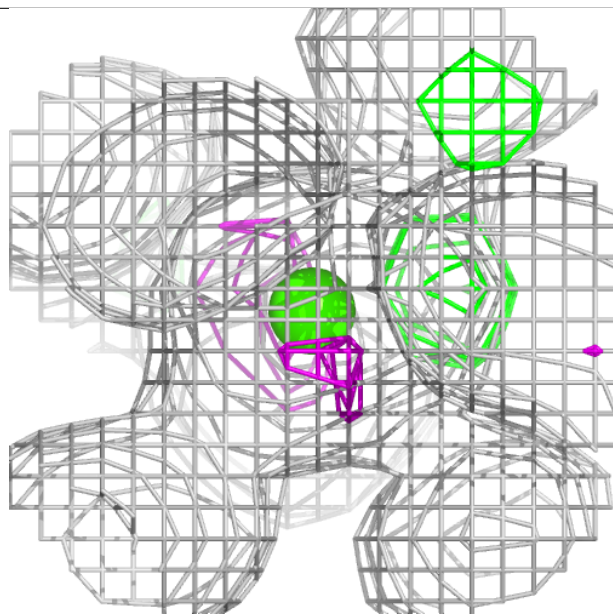
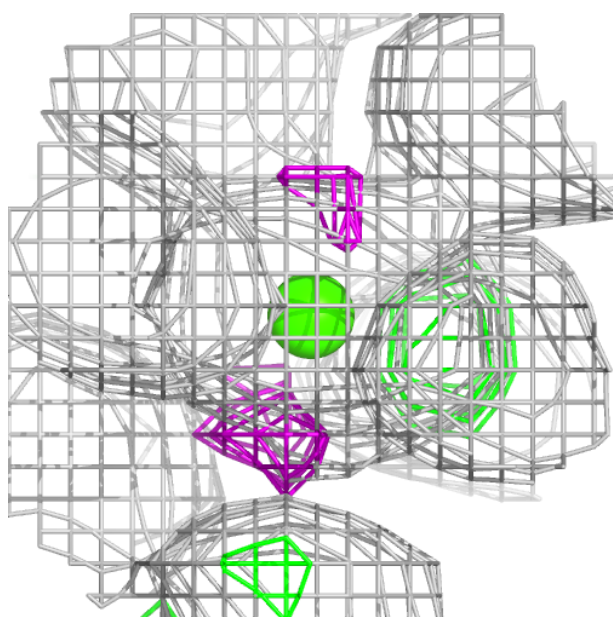
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	AAA	202	5/5	0.73	0.15	35,43,47,48	0
6	PEG	CCC	205	7/7	0.73	0.21	20,32,46,47	0
6	PEG	BBB	204	7/7	0.76	0.19	25,27,33,33	0
5	EDO	DDD	203	4/4	0.77	0.17	33,34,36,37	0
3	SO4	AAA	204	5/5	0.82	0.11	44,53,54,61	0
5	EDO	DDD	204	4/4	0.82	0.17	41,44,44,44	0
3	SO4	AAA	203	5/5	0.83	0.12	45,47,62,65	0
5	EDO	CCC	204	4/4	0.84	0.17	42,42,46,47	0
5	EDO	CCC	206	4/4	0.84	0.14	28,29,33,33	0
6	PEG	CCC	207	7/7	0.84	0.15	16,25,32,35	0
5	EDO	BBB	203	4/4	0.86	0.15	42,42,43,46	0
3	SO4	CCC	202	5/5	0.94	0.16	23,23,26,28	1
2	CA	AAA	201	1/1	0.96	0.06	19,19,19,19	0
4	MG	CCC	203	1/1	0.96	0.16	25,25,25,25	0
4	MG	DDD	202	1/1	0.97	0.23	25,25,25,25	0
4	MG	AAA	205	1/1	0.98	0.15	23,23,23,23	0
4	MG	BBB	202	1/1	0.98	0.15	16,16,16,16	0
2	CA	CCC	201	1/1	0.99	0.04	13,13,13,13	0
2	CA	DDD	201	1/1	0.99	0.03	13,13,13,13	0
2	CA	BBB	201	1/1	0.99	0.04	14,14,14,14	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.

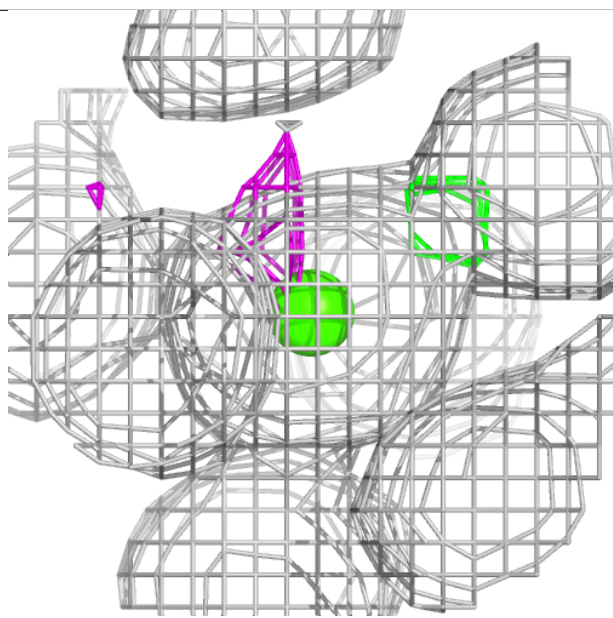
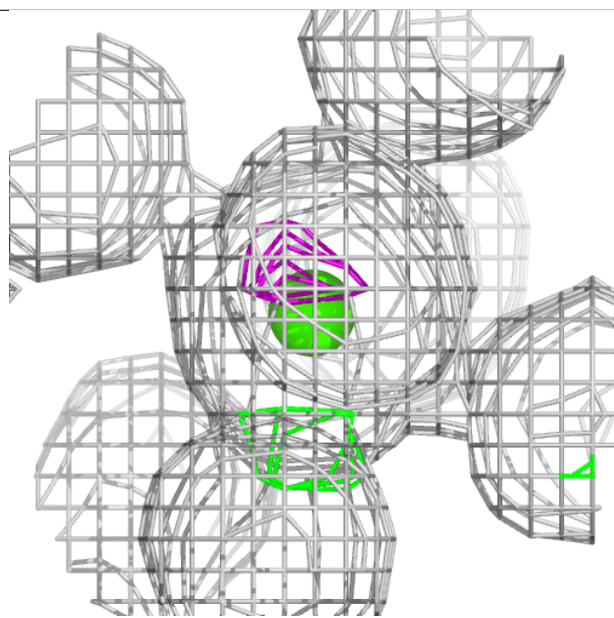
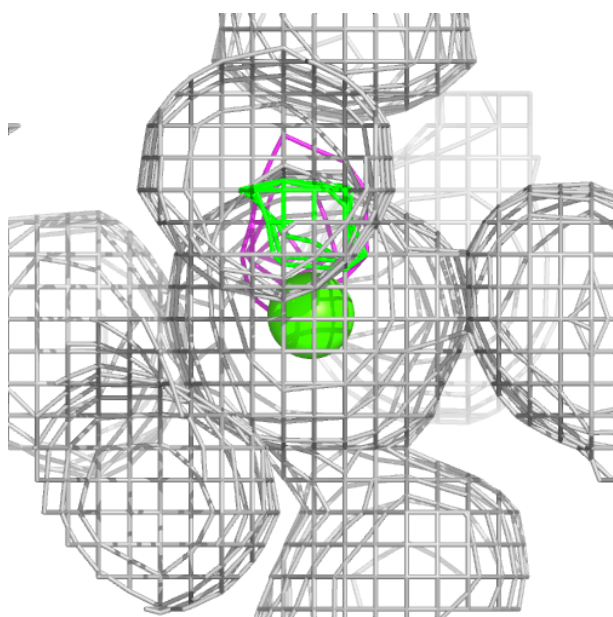
Electron density around CA AAA 201:

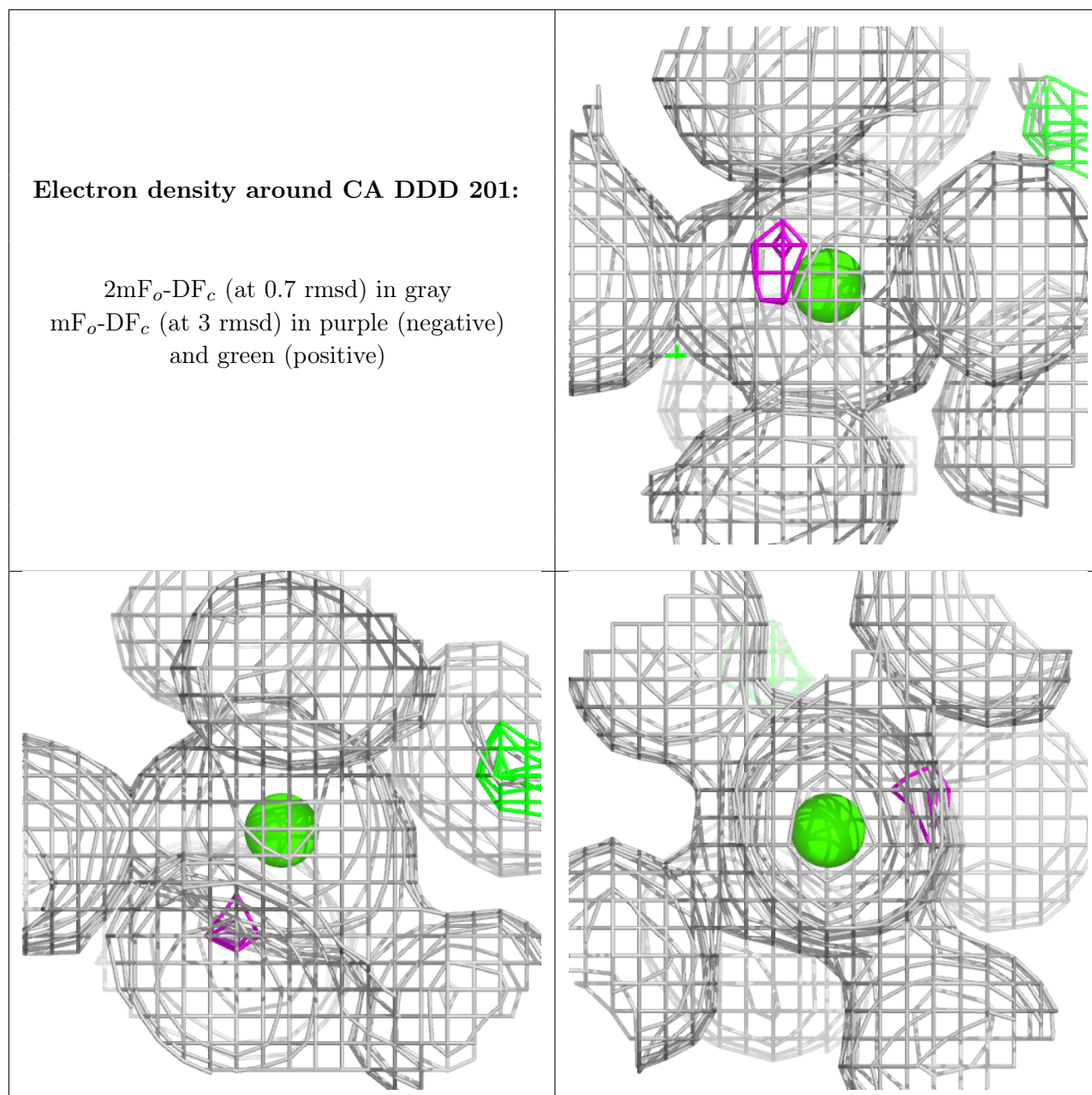
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

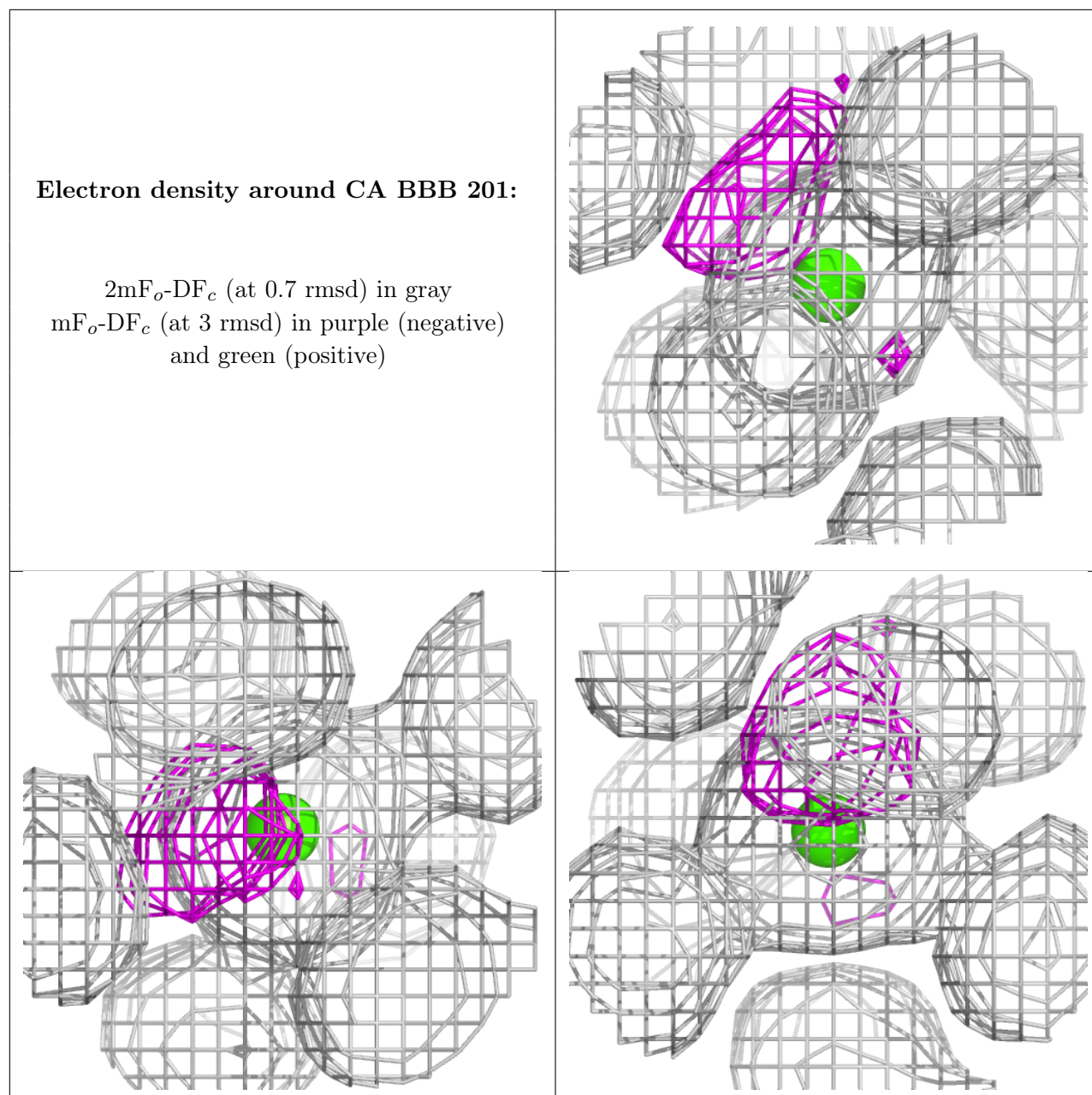


Electron density around CA CCC 201:

$2mF_o-DF_c$ (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.