Full wwPDB X-ray Structure Validation Report (i)

Jul 4, 2022 – 01:13 pm BST

PDB ID	:	7P1Y
Title	:	A small alarmone hydrolase TdActApo2 mutant - T78N
Authors	:	Jin, Y.; Roth, C.; Rizkallah, P.
Deposited on	:	2021-07-02
Resolution	:	2.38 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 (i) 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 (1)) were used in the production of this report:

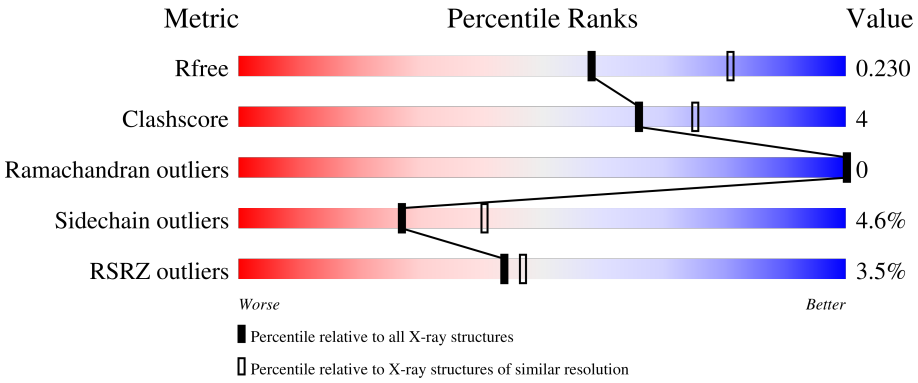
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.38 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	AAA	232	3% 66% 9% 25%
1	BBB	232	2% 65% 7% • 26%
1	CCC	232	3% 65% 8% 26%
1	DDD	232	3% 65% 7% • 26%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11244 atoms, of which 5635 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 HD domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	BBB	171	Total	C	H	N	O	S	32	0	0
			2761	879	1395	217	261	9			
1	DDD	172	Total	C	H	N	O	S	33	1	0
			2776	883	1402	219	263	9			
1	CCC	171	Total	C	H	N	O	S	33	1	0
			2782	884	1408	220	261	9			
1	AAA	174	Total	C	H	N	O	S	34	2	0
			2831	900	1430	225	266	10			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-26	MET	-	initiating methionine	UNP Q73M21
BBB	-25	GLY	-	expression tag	UNP Q73M21
BBB	-24	SER	-	expression tag	UNP Q73M21
BBB	-23	SER	-	expression tag	UNP Q73M21
BBB	-22	HIS	-	expression tag	UNP Q73M21
BBB	-21	HIS	-	expression tag	UNP Q73M21
BBB	-20	HIS	-	expression tag	UNP Q73M21
BBB	-19	HIS	-	expression tag	UNP Q73M21
BBB	-18	HIS	-	expression tag	UNP Q73M21
BBB	-17	HIS	-	expression tag	UNP Q73M21
BBB	-16	SER	-	expression tag	UNP Q73M21
BBB	-15	SER	-	expression tag	UNP Q73M21
BBB	-14	GLU	-	expression tag	UNP Q73M21
BBB	-13	ASN	-	expression tag	UNP Q73M21
BBB	-12	LEU	-	expression tag	UNP Q73M21
BBB	-11	TYR	-	expression tag	UNP Q73M21
BBB	-10	PHE	-	expression tag	UNP Q73M21
BBB	-9	GLN	-	expression tag	UNP Q73M21
BBB	-8	GLY	-	expression tag	UNP Q73M21
BBB	-7	GLY	-	expression tag	UNP Q73M21
BBB	-6	LEU	-	expression tag	UNP Q73M21

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-5	VAL	-	expression tag	UNP Q73M21
BBB	-4	PRO	-	expression tag	UNP Q73M21
BBB	-3	ARG	-	expression tag	UNP Q73M21
BBB	-2	GLY	-	expression tag	UNP Q73M21
BBB	-1	SER	-	expression tag	UNP Q73M21
BBB	0	HIS	-	expression tag	UNP Q73M21
BBB	78	ASN	ASP	engineered mutation	UNP Q73M21
DDD	-26	MET	-	initiating methionine	UNP Q73M21
DDD	-25	GLY	-	expression tag	UNP Q73M21
DDD	-24	SER	-	expression tag	UNP Q73M21
DDD	-23	SER	-	expression tag	UNP Q73M21
DDD	-22	HIS	-	expression tag	UNP Q73M21
DDD	-21	HIS	-	expression tag	UNP Q73M21
DDD	-20	HIS	-	expression tag	UNP Q73M21
DDD	-19	HIS	-	expression tag	UNP Q73M21
DDD	-18	HIS	-	expression tag	UNP Q73M21
DDD	-17	HIS	-	expression tag	UNP Q73M21
DDD	-16	SER	-	expression tag	UNP Q73M21
DDD	-15	SER	-	expression tag	UNP Q73M21
DDD	-14	GLU	-	expression tag	UNP Q73M21
DDD	-13	ASN	-	expression tag	UNP Q73M21
DDD	-12	LEU	-	expression tag	UNP Q73M21
DDD	-11	TYR	-	expression tag	UNP Q73M21
DDD	-10	PHE	-	expression tag	UNP Q73M21
DDD	-9	GLN	-	expression tag	UNP Q73M21
DDD	-8	GLY	-	expression tag	UNP Q73M21
DDD	-7	GLY	-	expression tag	UNP Q73M21
DDD	-6	LEU	-	expression tag	UNP Q73M21
DDD	-5	VAL	-	expression tag	UNP Q73M21
DDD	-4	PRO	-	expression tag	UNP Q73M21
DDD	-3	ARG	-	expression tag	UNP Q73M21
DDD	-2	GLY	-	expression tag	UNP Q73M21
DDD	-1	SER	-	expression tag	UNP Q73M21
DDD	0	HIS	-	expression tag	UNP Q73M21
DDD	78	ASN	ASP	engineered mutation	UNP Q73M21
CCC	-26	MET	-	initiating methionine	UNP Q73M21
CCC	-25	GLY	-	expression tag	UNP Q73M21
CCC	-24	SER	-	expression tag	UNP Q73M21
CCC	-23	SER	-	expression tag	UNP Q73M21
CCC	-22	HIS	-	expression tag	UNP Q73M21
CCC	-21	HIS	-	expression tag	UNP Q73M21
CCC	-20	HIS	-	expression tag	UNP Q73M21

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-19	HIS	-	expression tag	UNP Q73M21
CCC	-18	HIS	-	expression tag	UNP Q73M21
CCC	-17	HIS	-	expression tag	UNP Q73M21
CCC	-16	SER	-	expression tag	UNP Q73M21
CCC	-15	SER	-	expression tag	UNP Q73M21
CCC	-14	GLU	-	expression tag	UNP Q73M21
CCC	-13	ASN	-	expression tag	UNP Q73M21
CCC	-12	LEU	-	expression tag	UNP Q73M21
CCC	-11	TYR	-	expression tag	UNP Q73M21
CCC	-10	PHE	-	expression tag	UNP Q73M21
CCC	-9	GLN	-	expression tag	UNP Q73M21
CCC	-8	GLY	-	expression tag	UNP Q73M21
CCC	-7	GLY	-	expression tag	UNP Q73M21
CCC	-6	LEU	-	expression tag	UNP Q73M21
CCC	-5	VAL	-	expression tag	UNP Q73M21
CCC	-4	PRO	-	expression tag	UNP Q73M21
CCC	-3	ARG	-	expression tag	UNP Q73M21
CCC	-2	GLY	-	expression tag	UNP Q73M21
CCC	-1	SER	-	expression tag	UNP Q73M21
CCC	0	HIS	-	expression tag	UNP Q73M21
CCC	78	ASN	ASP	engineered mutation	UNP Q73M21
AAA	-26	MET	-	initiating methionine	UNP Q73M21
AAA	-25	GLY	-	expression tag	UNP Q73M21
AAA	-24	SER	-	expression tag	UNP Q73M21
AAA	-23	SER	-	expression tag	UNP Q73M21
AAA	-22	HIS	-	expression tag	UNP Q73M21
AAA	-21	HIS	-	expression tag	UNP Q73M21
AAA	-20	HIS	-	expression tag	UNP Q73M21
AAA	-19	HIS	-	expression tag	UNP Q73M21
AAA	-18	HIS	-	expression tag	UNP Q73M21
AAA	-17	HIS	-	expression tag	UNP Q73M21
AAA	-16	SER	-	expression tag	UNP Q73M21
AAA	-15	SER	-	expression tag	UNP Q73M21
AAA	-14	GLU	-	expression tag	UNP Q73M21
AAA	-13	ASN	-	expression tag	UNP Q73M21
AAA	-12	LEU	-	expression tag	UNP Q73M21
AAA	-11	TYR	-	expression tag	UNP Q73M21
AAA	-10	PHE	-	expression tag	UNP Q73M21
AAA	-9	GLN	-	expression tag	UNP Q73M21
AAA	-8	GLY	-	expression tag	UNP Q73M21
AAA	-7	GLY	-	expression tag	UNP Q73M21
AAA	-6	LEU	-	expression tag	UNP Q73M21

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-5	VAL	-	expression tag	UNP Q73M21
AAA	-4	PRO	-	expression tag	UNP Q73M21
AAA	-3	ARG	-	expression tag	UNP Q73M21
AAA	-2	GLY	-	expression tag	UNP Q73M21
AAA	-1	SER	-	expression tag	UNP Q73M21
AAA	0	HIS	-	expression tag	UNP Q73M21
AAA	78	ASN	ASP	engineered mutation	UNP Q73M21

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	CCC	1	Total Cl 1 1	0	0
3	AAA	1	Total Cl 1 1	0	0

- Molecule 4 is water.

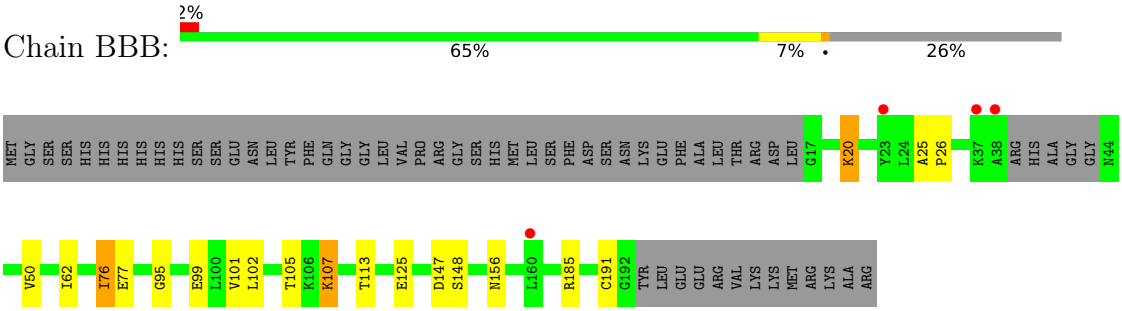
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	16	Total O 16 16	0	0
4	DDD	16	Total O 17 17	0	1
4	CCC	22	Total O 22 22	0	0
4	AAA	33	Total O 33 33	0	0

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.

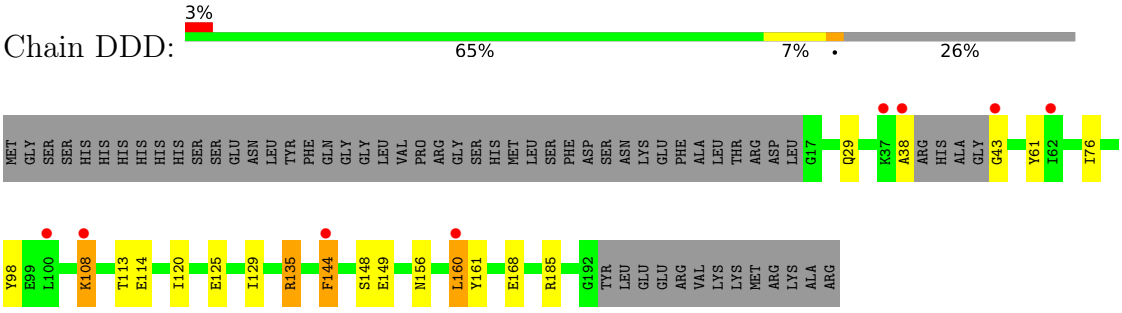
• Molecule 1: HD domain-containing protein

Chain BBB:



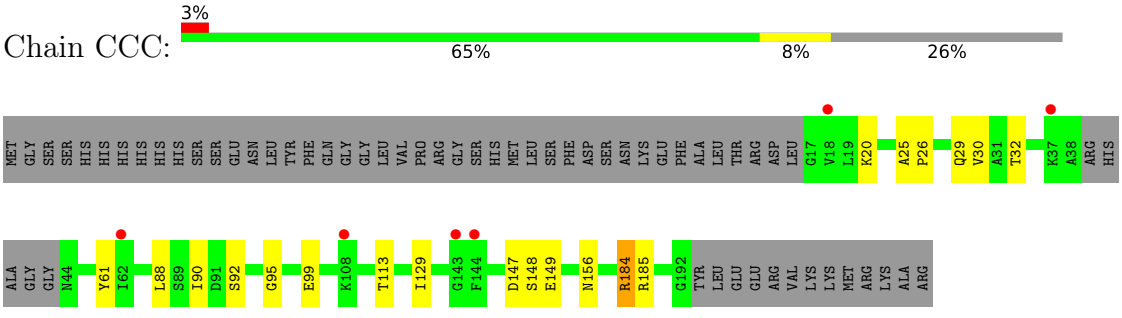
• Molecule 1: HD domain-containing protein

Chain DDD:



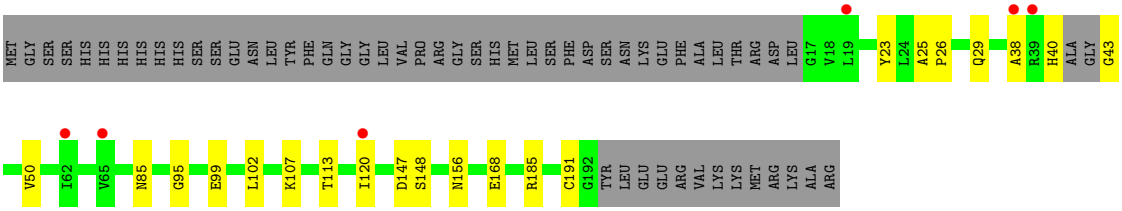
• Molecule 1: HD domain-containing protein

Chain CCC:



• Molecule 1: HD domain-containing protein

Chain AAA:


MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLU ASN LEU TYR PHE GLN GLY GLY LEU VAL PRO ARG GLY SER HIS MET LEU SER PHE ASP SER ASN LYS GLU PHE ALA LEU THR ARG ASP LEU G17 V18 L19 Y23 L24 A25 P26 Q29 A38 R39 H40 ALA GLY G43
V50 I62 V65 N85 G95 E99 L102 K107 T113 I120 D147 S148 N156 E168 R185 C191 G192 TYR LEU GLU GLU ARG VAL LYS LYS MET ARG LYS ALA ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.29Å 69.19Å 132.07Å 90.00° 93.02° 90.00°	Depositor
Resolution (Å)	61.28 – 2.38 61.27 – 2.38	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.28-2.38) 100.0 (61.27-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.191 , 0.227 0.199 , 0.230	Depositor DCC
R_{free} test set	2212 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11244	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: MN, CL

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	0.75	0/1426	0.86	0/1918
1	BBB	0.73	0/1384	0.87	0/1863
1	CCC	0.77	0/1395	0.89	0/1877
1	DDD	0.75	0/1392	0.85	0/1873
All	All	0.75	0/5597	0.87	0/7531

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	AAA	1401	1430	1427	11	0
1	BBB	1366	1395	1391	17	0
1	CCC	1374	1408	1405	10	0
1	DDD	1374	1402	1396	11	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	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CCC	1	0	0	0	0
4	AAA	33	0	0	1	0
4	BBB	16	0	0	0	0
4	CCC	22	0	0	0	0
4	DDD	17	0	0	1	0
All	All	5609	5635	5619	45	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 4.

All (45) 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:CCC:29:GLN:O	1:CCC:32:THR:HB	1.83	0.79
1:CCC:30:VAL:HG21	1:CCC:90:ILE:HD11	1.63	0.78
1:CCC:88:LEU:HD13	1:AAA:85:ASN:HB2	1.71	0.71
1:BBB:76:ILE:HD13	1:BBB:77:GLU:N	2.05	0.71
1:AAA:120:ILE:HD11	1:AAA:168:GLU:OE2	1.97	0.64
1:BBB:25:ALA:N	1:BBB:26:PRO:HD2	2.14	0.62
1:DDD:120:ILE:HD11	1:DDD:168:GLU:OE1	2.01	0.61
1:DDD:108:LYS:HD2	4:AAA:432:HOH:O	2.02	0.58
1:BBB:76:ILE:CD1	1:BBB:77:GLU:N	2.67	0.57
1:CCC:92:SER:O	1:AAA:102:LEU:HD21	2.05	0.57
1:BBB:20:LYS:O	1:AAA:23:TYR:OH	2.20	0.57
1:BBB:76:ILE:CD1	1:BBB:77:GLU:H	2.18	0.56
1:BBB:76:ILE:HD11	1:BBB:105:THR:OG1	2.07	0.53
1:BBB:95:GLY:O	1:BBB:99:GLU:HG2	2.09	0.53
1:DDD:156:ASN:OD1	1:DDD:185:ARG:NH2	2.42	0.52
1:CCC:95:GLY:O	1:CCC:99:GLU:HG2	2.10	0.52
1:DDD:76:ILE:HD11	1:DDD:98:TYR:HE1	1.77	0.50
1:AAA:156:ASN:OD1	1:AAA:185:ARG:NH2	2.44	0.49
1:AAA:95:GLY:O	1:AAA:99:GLU:HG2	2.11	0.49
1:CCC:156:ASN:OD1	1:CCC:185:ARG:NH2	2.44	0.49
1:BBB:107:LYS:HA	1:BBB:107:LYS:CE	2.43	0.49
1:DDD:135:ARG:HD3	4:DDD:403:HOH:O	2.12	0.49
1:DDD:76:ILE:HD11	1:DDD:98:TYR:CE1	2.47	0.49
1:BBB:156:ASN:OD1	1:BBB:185:ARG:NH2	2.46	0.48
1:AAA:38:ALA:HA	1:AAA:43:GLY:O	2.13	0.47
1:DDD:144:PHE:CD1	1:DDD:144:PHE:N	2.83	0.47
1:DDD:38:ALA:HA	1:DDD:43[B]:GLY:O	2.15	0.46
1:DDD:38:ALA:HA	1:DDD:43[A]:GLY:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:76:ILE:HG13	1:BBB:101:VAL:CG1	2.48	0.44
1:BBB:76:ILE:HD12	1:BBB:76:ILE:N	2.35	0.42
1:BBB:147:ASP:O	1:BBB:147:ASP:OD1	2.38	0.42
1:BBB:62:ILE:HG13	1:BBB:62:ILE:O	2.20	0.42
1:BBB:50:VAL:HG12	1:AAA:50:VAL:HG12	2.02	0.41
1:CCC:147:ASP:OD1	1:CCC:147:ASP:O	2.39	0.41
1:BBB:102:LEU:HD23	1:BBB:102:LEU:HA	1.92	0.41
1:DDD:160:LEU:HD22	1:DDD:161:TYR:CZ	2.55	0.41
1:AAA:102:LEU:HD23	1:AAA:102:LEU:HA	1.92	0.41
1:CCC:61:TYR:CE1	1:CCC:129:ILE:HD13	2.56	0.41
1:AAA:147:ASP:O	1:AAA:147:ASP:OD1	2.39	0.41
1:AAA:25:ALA:N	1:AAA:26:PRO:CD	2.84	0.41
1:BBB:76:ILE:HD12	1:BBB:76:ILE:H	1.86	0.40
1:DDD:61:TYR:CE1	1:DDD:129:ILE:HD13	2.57	0.40
1:CCC:25:ALA:N	1:CCC:26:PRO:CD	2.85	0.40
1:BBB:76:ILE:HD13	1:BBB:77:GLU:H	1.76	0.40

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	172/232 (74%)	166 (96%)	6 (4%)	0	100	100
1	BBB	167/232 (72%)	158 (95%)	9 (5%)	0	100	100
1	CCC	168/232 (72%)	161 (96%)	7 (4%)	0	100	100
1	DDD	168/232 (72%)	163 (97%)	5 (3%)	0	100	100
All	All	675/928 (73%)	648 (96%)	27 (4%)	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	156/204 (76%)	150 (96%)	6 (4%)	33	49
1	BBB	152/204 (74%)	145 (95%)	7 (5%)	27	40
1	CCC	153/204 (75%)	147 (96%)	6 (4%)	32	48
1	DDD	152/204 (74%)	142 (93%)	10 (7%)	16	24
All	All	613/816 (75%)	584 (95%)	29 (5%)	27	39

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	20	LYS
1	BBB	76	ILE
1	BBB	107	LYS
1	BBB	113	THR
1	BBB	125	GLU
1	BBB	148	SER
1	BBB	191	CYS
1	DDD	29	GLN
1	DDD	108	LYS
1	DDD	113	THR
1	DDD	114	GLU
1	DDD	125	GLU
1	DDD	135	ARG
1	DDD	144	PHE
1	DDD	148	SER
1	DDD	149	GLU
1	DDD	160	LEU
1	CCC	20	LYS
1	CCC	113	THR
1	CCC	148	SER
1	CCC	149	GLU
1	CCC	184[B]	ARG
1	CCC	184[C]	ARG
1	AAA	29	GLN

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Mol	Chain	Res	Type
1	AAA	40	HIS
1	AAA	107	LYS
1	AAA	113	THR
1	AAA	148	SER
1	AAA	191	CYS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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 (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	AAA	174/232 (75%)	0.74	6 (3%)	45	48	43, 59, 100, 149	0
1	BBB	171/232 (73%)	0.74	4 (2%)	60	62	44, 68, 105, 124	0
1	CCC	171/232 (73%)	0.67	6 (3%)	44	47	38, 58, 109, 137	1 (0%)
1	DDD	172/232 (74%)	0.75	8 (4%)	31	34	44, 63, 108, 139	1 (0%)
All	All	688/928 (74%)	0.72	24 (3%)	44	47	38, 62, 108, 149	2 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	144	PHE	5.2
1	DDD	144	PHE	4.9
1	BBB	23	TYR	3.0
1	DDD	62	ILE	3.0
1	DDD	37	LYS	3.0
1	AAA	62	ILE	2.9
1	DDD	43[A]	GLY	2.9
1	DDD	108	LYS	2.8
1	BBB	160	LEU	2.7
1	CCC	108	LYS	2.6
1	CCC	37	LYS	2.4
1	AAA	39	ARG	2.4
1	AAA	65	VAL	2.4
1	AAA	19	LEU	2.4
1	DDD	38	ALA	2.3
1	DDD	160	LEU	2.3
1	BBB	37	LYS	2.3
1	CCC	18	VAL	2.2
1	AAA	38	ALA	2.2
1	DDD	100	LEU	2.2
1	CCC	62	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	CCC	143	GLY	2.1
1	AAA	120	ILE	2.1
1	BBB	38	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

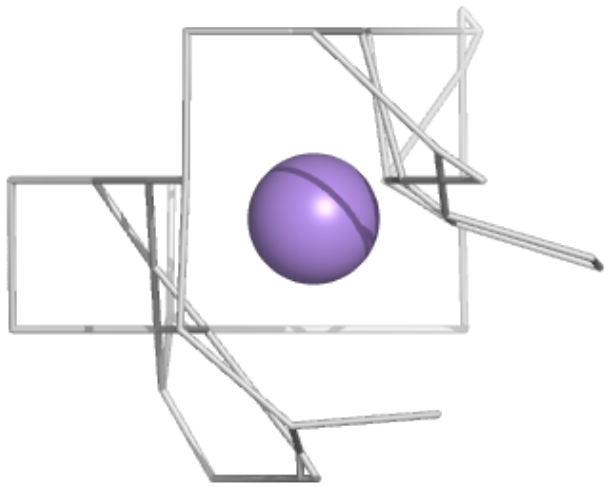
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

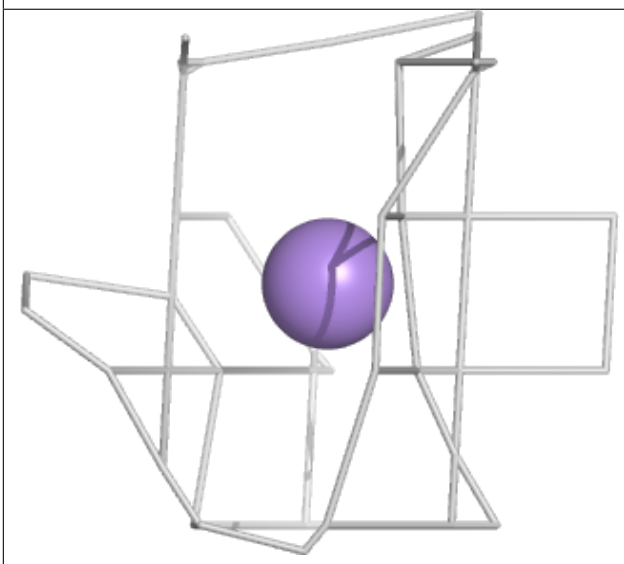
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	BBB	301	1/1	0.92	0.16	85,85,85,85	1
2	MN	DDD	301	1/1	0.93	0.07	72,72,72,72	1
2	MN	CCC	302	1/1	0.95	0.08	65,65,65,65	1
2	MN	AAA	302	1/1	0.96	0.09	66,66,66,66	1
3	CL	AAA	301	1/1	0.97	0.09	81,81,81,81	0
3	CL	CCC	301	1/1	1.00	0.16	48,48,48,48	0

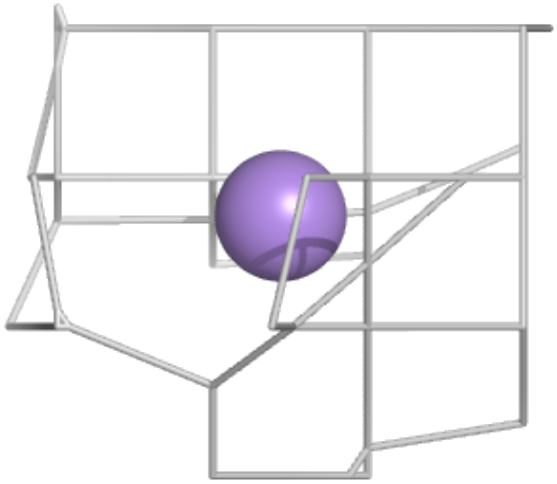
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MN BBB 301:

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

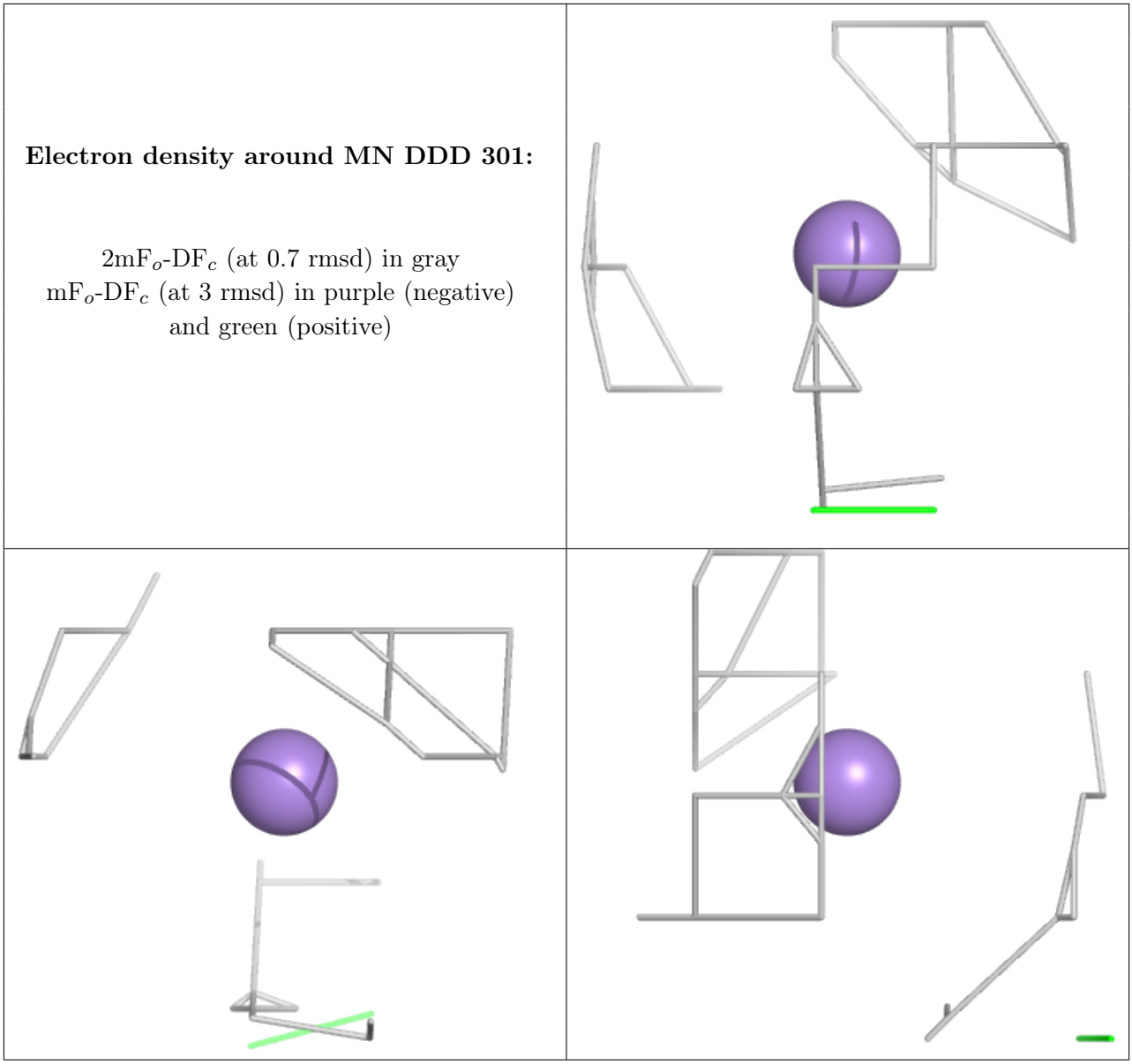






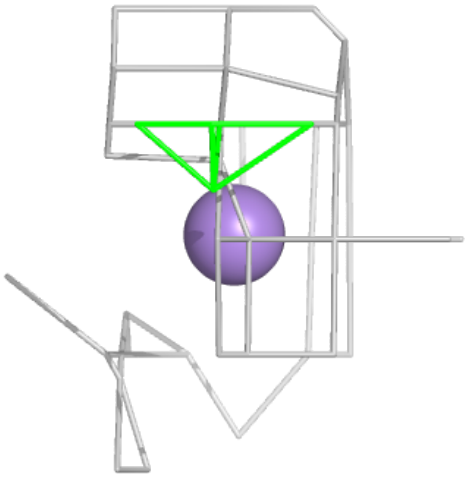
Electron density around MN DDD 301:

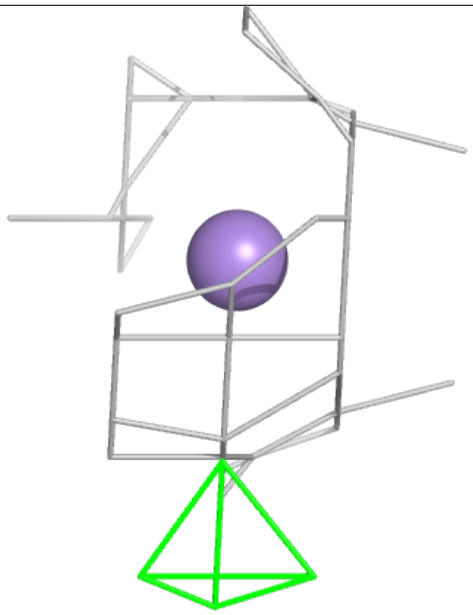
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

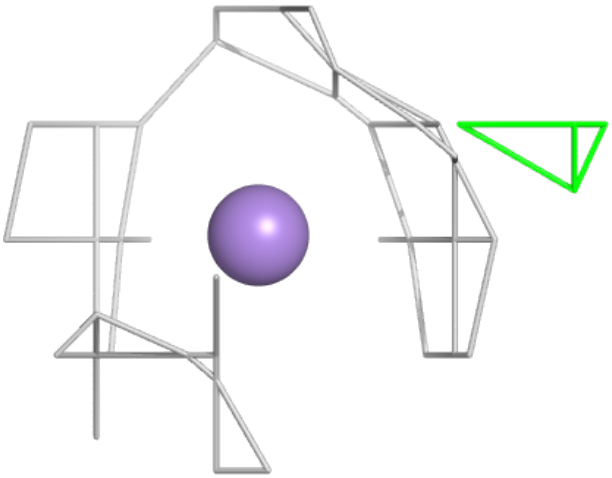


Electron density around MN CCC 302:

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

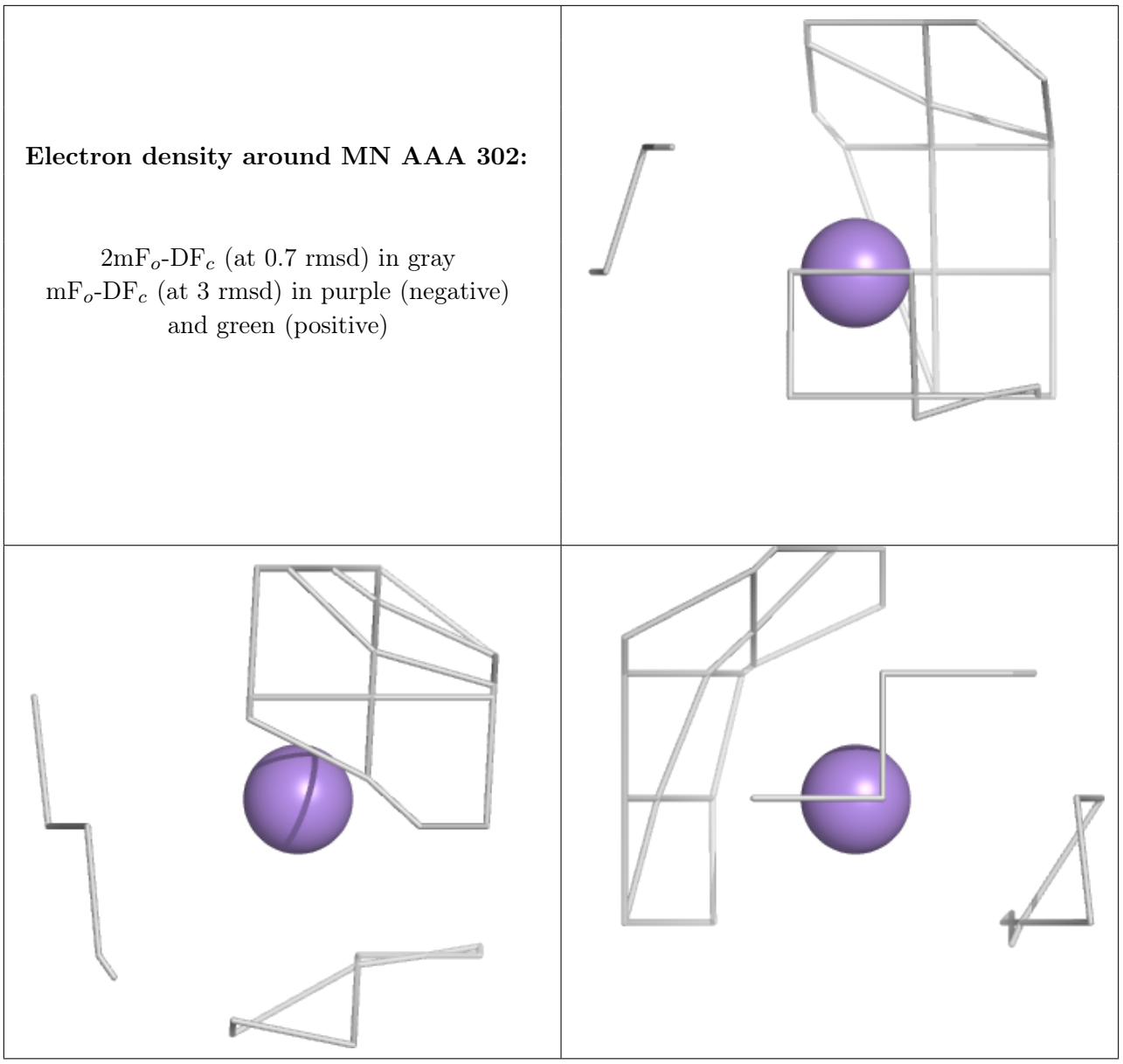






Electron density around MN AAA 302:

$2mF_o$-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 (i)

There are no such residues in this entry.