

wwPDB X-ray Structure Validation Summary Report (i)

Apr 2, 2024 – 02:10 PM JST

PDB ID : 8YUD

Title : Crystal structure of Xylose isomerase from Streptomyces avermitilis

Authors : Nam, K.H. Deposited on : 2024-03-27

Resolution : 2.81 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 (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:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ Xtriage \left(Phenix\right) & : & 1.13 \end{array}$

EDS : 2.36 buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)
oteins) : Engh & Huber (200)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

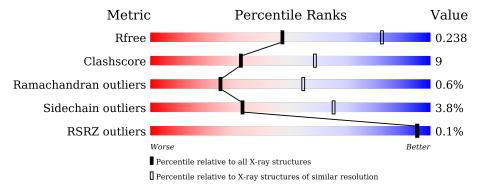
 $\begin{tabular}{lll} Validation Pipeline (wwPDB-VP) & : & 2.36 \end{tabular}$

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 2.81 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	Similar resolution
WIGHT	$(\# {\rm Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	388	78%	20%	
1	В	388	80%	20%	
1	С	388	79%	19%	
1	D	388	71%	26%	
1	Е	388	73%	24%	
1	F	388	75%	23%	



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18090 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 Xylose isomerase.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	A	386	Total	С	N	О	S	0	0	0
1	Λ	360	3013	1901	539	565	8	0	0	
1	В	386	Total	С	N	О	S	0	0	0
1	Ъ	360	3013	1901	539	565	8	0	0	
1	С	386	Total	С	N	О	S	0	0	0
1		360	3013	1901	539	565	8	0	0	
1	D	386	Total	С	N	О	S	0	0	0
1	D	360	3013	1901	539	565	8	0	0	
1	Е	386	Total	С	N	Ο	S	0	0	0
1	ш	300	3013	1901	539	565	8	0	U	0
1	F	386	Total	С	N	О	S	0	0	0
1	I'	360	3013	1901	539	565	8	U	U	U

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

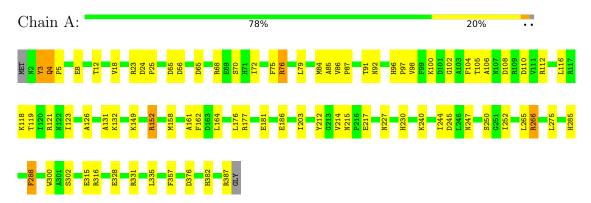
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	В	2	Total Mg 2 2	0	0
2	С	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	F	2	Total Mg 2 2	0	0



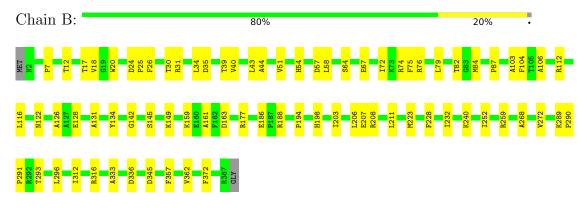
3 Residue-property plots (i)

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.

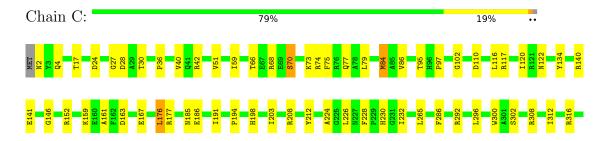
• Molecule 1: Xylose isomerase



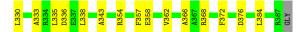
• Molecule 1: Xylose isomerase



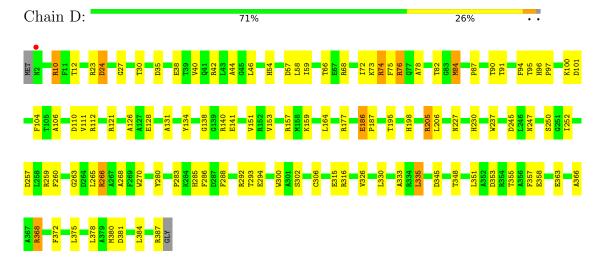
• Molecule 1: Xylose isomerase



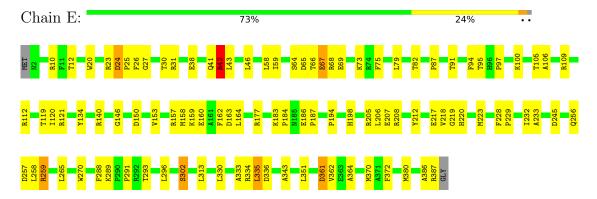




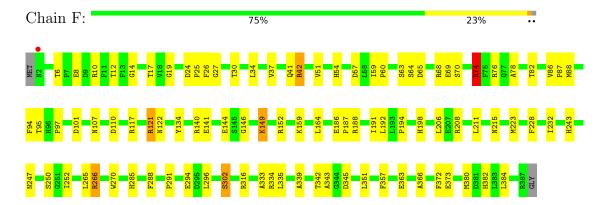
 \bullet Molecule 1: Xylose isomerase



• Molecule 1: Xylose isomerase



• Molecule 1: Xylose isomerase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	129.13Å 129.13Å 233.06Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.21 - 2.81	Depositor
Resolution (A)	34.21 - 2.81	EDS
% Data completeness	97.5 (34.21-2.81)	Depositor
(in resolution range)	97.5 (34.21-2.81)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.41 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
D.D.	0.187 , 0.243	Depositor
R, R_{free}	0.186 , 0.238	DCC
R_{free} test set	1994 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 17.0	EDS
L-test for twinning ²	$< L > = 0.46, < L^2> = 0.29$	Xtriage
Estimated twinning fraction	0.115 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18090	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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

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	Mol Chain		lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.47	0/3084	0.72	2/4181~(0.0%)	
1	В	0.46	0/3084	0.70	0/4181	
1	С	0.46	0/3084	0.70	1/4181 (0.0%)	
1	D	0.45	0/3084	0.72	1/4181~(0.0%)	
1	Е	0.44	0/3084	0.72	1/4181 (0.0%)	
1	F	0.47	0/3084	0.70	0/4181	
All	All	0.46	0/18504	0.71	5/25086~(0.0%)	

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	A	0	2
1	D	0	6
1	Е	0	1
1	F	0	6
All	All	0	15

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	D	24	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	265	LEU	CB-CG-CD2	-5.43	101.76	111.00
1	Е	24	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	3	TYR	CB-CG-CD1	5.09	124.05	121.00
1	С	24	ASP	CB-CG-OD1	5.05	122.84	118.30



There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	ARG	Sidechain
1	A	76	ARG	Sidechain
1	D	10	ARG	Sidechain
1	D	74	ARG	Sidechain
1	D	76	ARG	Sidechain

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	3013	0	2907	45	0
1	В	3013	0	2907	44	0
1	С	3013	0	2907	53	0
1	D	3013	0	2907	79	0
1	Е	3013	0	2907	72	0
1	F	3013	0	2907	69	0
2	A	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0
2	Е	2	0	0	0	0
2	F	2	0	0	0	0
All	All	18090	0	17442	311	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 9.

The worst 5 of 311 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	Clash overlap (Å)
1:D:195:THR:HG1	1:D:198:HIS:HD1	0.98	0.94
1:E:38:GLU:OE2	1:E:42:ARG:NH1	2.08	0.87
1:F:19:GLY:HA2	1:F:34:LEU:HD12	1.57	0.87
1:E:91:THR:HG1	1:E:134:TYR:HH	1.20	0.81

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Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$	
1:B:40:VAL:HG13	1:B:84:MET:HG3	1.63	0.80	

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	Perce	entiles
1	A	384/388~(99%)	363 (94%)	19 (5%)	2 (0%)	29	59
1	В	384/388~(99%)	367 (96%)	14 (4%)	3 (1%)	19	47
1	С	384/388 (99%)	363 (94%)	19 (5%)	2 (0%)	29	59
1	D	384/388 (99%)	366 (95%)	16 (4%)	2 (0%)	29	59
1	E	384/388~(99%)	364 (95%)	18 (5%)	2 (0%)	29	59
1	F	384/388 (99%)	358 (93%)	24 (6%)	2 (0%)	29	59
All	All	2304/2328 (99%)	2181 (95%)	110 (5%)	13 (1%)	25	54

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	186	GLU
1	A	357	PHE
1	Е	186	GLU
1	F	186	GLU
1	A	186	GLU

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	${\rm sidechain}$	conformation	was
analysed, and the total	number of	residues	S.						

Mol	Chain	Analysed	Rotameric	Outliers	Percentile	es
1	A	$297/298\ (100\%)$	282 (95%)	15 (5%)	24 54	
1	В	$297/298\ (100\%)$	291 (98%)	6 (2%)	55 83	
1	\mathbf{C}	$297/298\ (100\%)$	289 (97%)	8 (3%)	44 77	
1	D	$297/298\ (100\%)$	285 (96%)	12 (4%)	31 64	
1	E	$297/298\ (100\%)$	283 (95%)	14 (5%)	26 57	
1	F	$297/298\ (100\%)$	285 (96%)	12 (4%)	31 64	
All	All	1782/1788 (100%)	1715 (96%)	67 (4%)	33 65	

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	74	ARG
1	F	121	ARG
1	F	335	LEU
1	С	141	GLU
1	С	84	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	Ε	215	ASN
1	Е	243	HIS
1	Ε	382	HIS
1	A	230	HIS
1	В	2	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 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, 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>	# RSRZ > 2		$OWAB(A^2)$	Q < 0.9
1	A	$386/388 \ (99\%)$	-0.37	0 100	100	21, 32, 45, 70	0
1	В	386/388 (99%)	-0.36	0 100	100	22, 33, 45, 71	0
1	С	386/388 (99%)	-0.32	0 100	100	22, 34, 47, 70	0
1	D	386/388 (99%)	-0.32	1 (0%)	94 93	24, 36, 47, 85	0
1	E	386/388 (99%)	-0.32	0 100	100	24, 35, 48, 75	0
1	F	386/388 (99%)	-0.26	1 (0%)	94 93	24, 38, 52, 83	0
All	All	2316/2328 (99%)	-0.32	2 (0%)	95 95	21, 34, 48, 85	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	ASN	3.4
1	F	2	ASN	2.5

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)

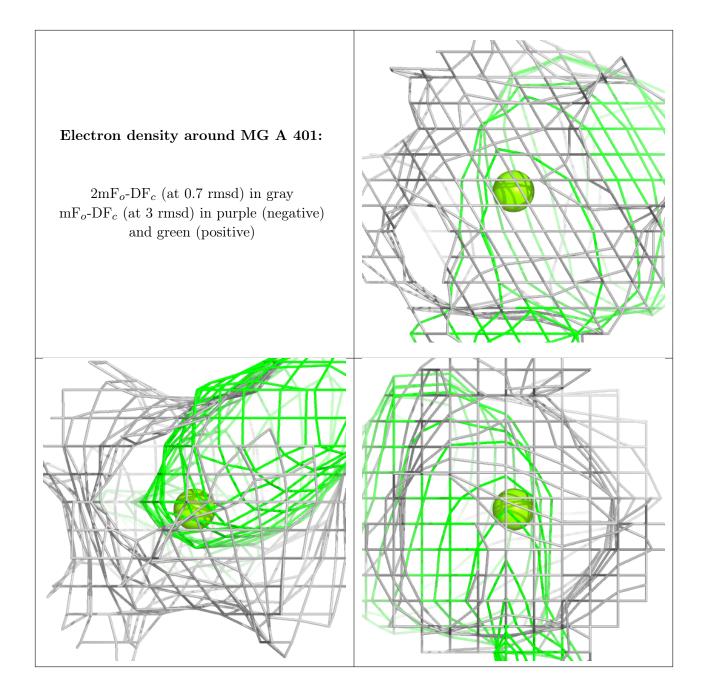
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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



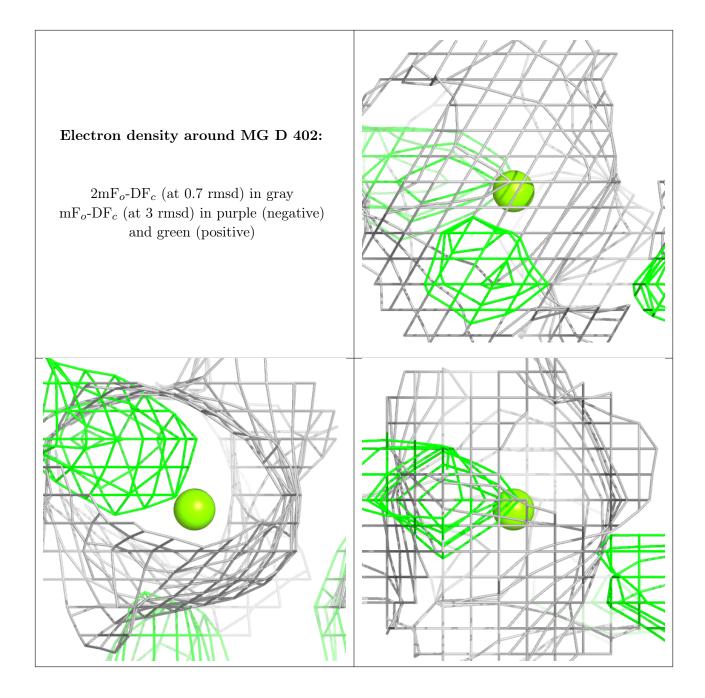
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	MG	A	401	1/1	0.79	0.23	38,38,38,38	0
2	MG	D	402	1/1	0.83	0.16	33,33,33,33	0
2	MG	Е	402	1/1	0.85	0.20	44,44,44	0
2	MG	F	402	1/1	0.85	0.24	42,42,42,42	0
2	MG	F	401	1/1	0.88	0.14	29,29,29,29	0
2	MG	В	402	1/1	0.89	0.19	36,36,36,36	0
2	MG	С	401	1/1	0.90	0.16	37,37,37,37	0
2	MG	A	402	1/1	0.91	0.17	40,40,40,40	0
2	MG	С	402	1/1	0.92	0.17	35,35,35,35	0
2	MG	Е	401	1/1	0.94	0.11	32,32,32,32	0
2	MG	В	401	1/1	0.94	0.17	38,38,38,38	0
2	MG	D	401	1/1	0.96	0.10	35,35,35,35	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.

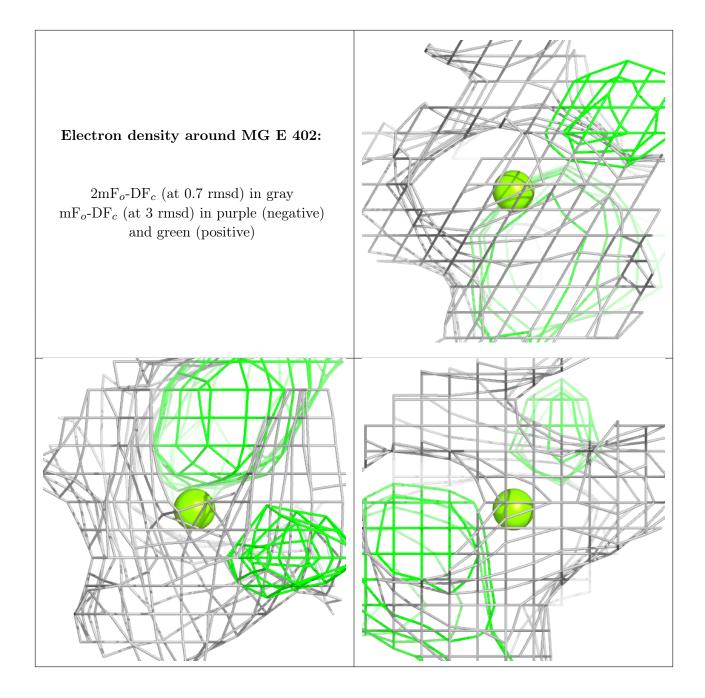




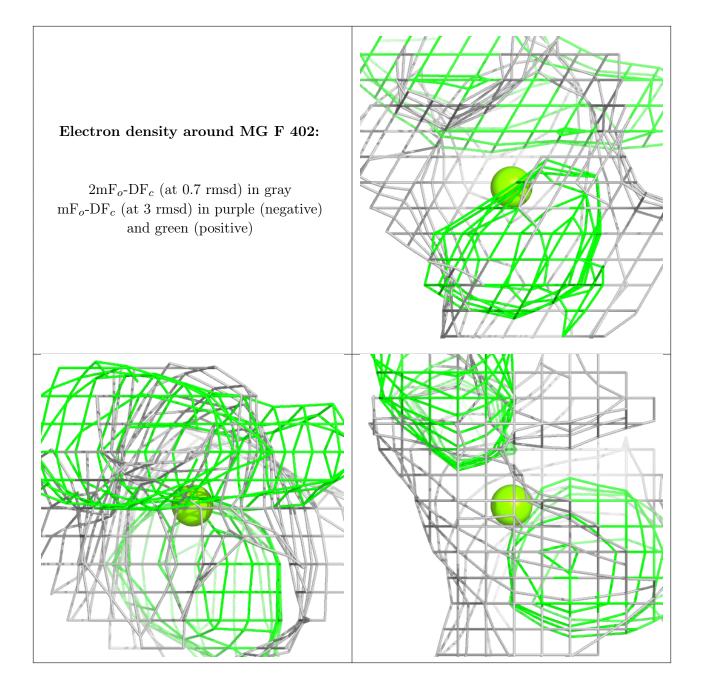




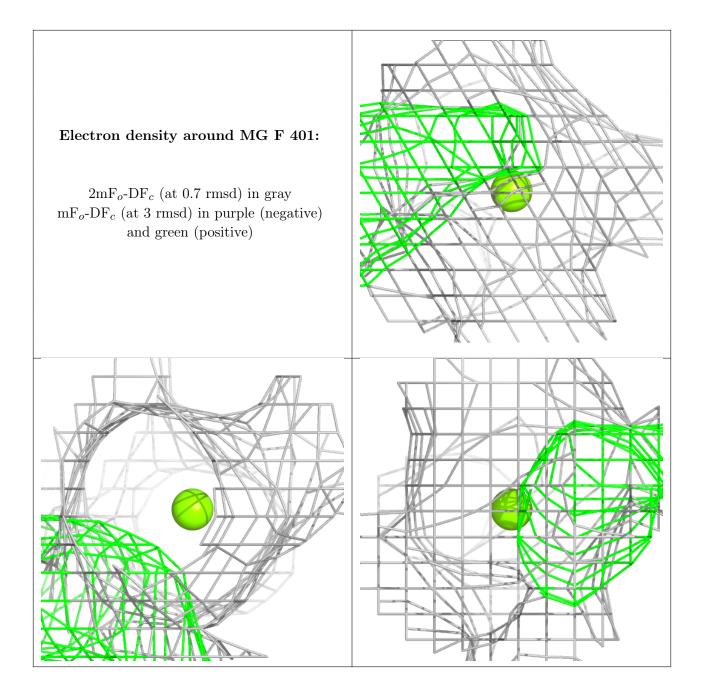




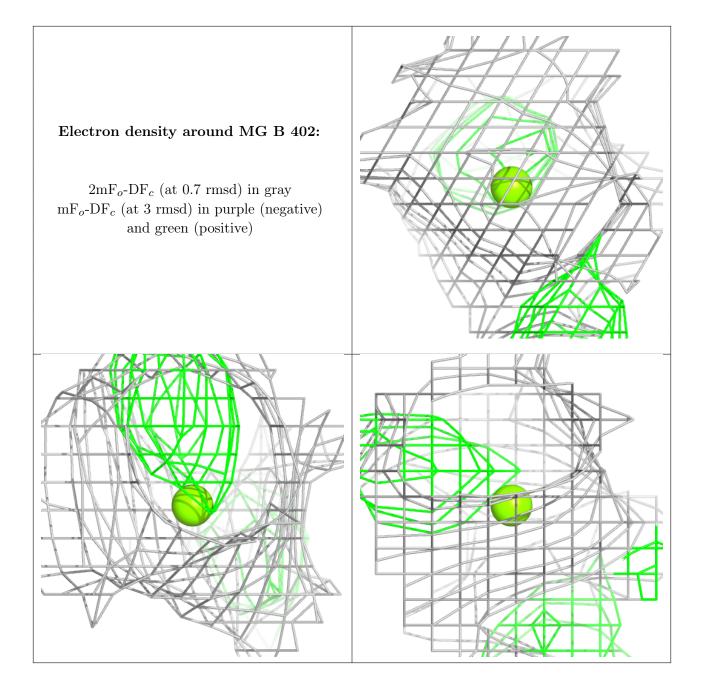




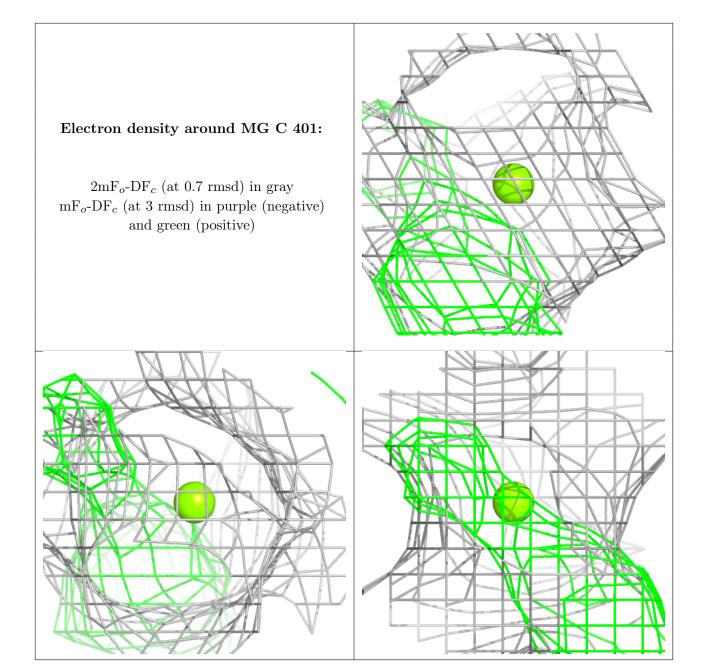




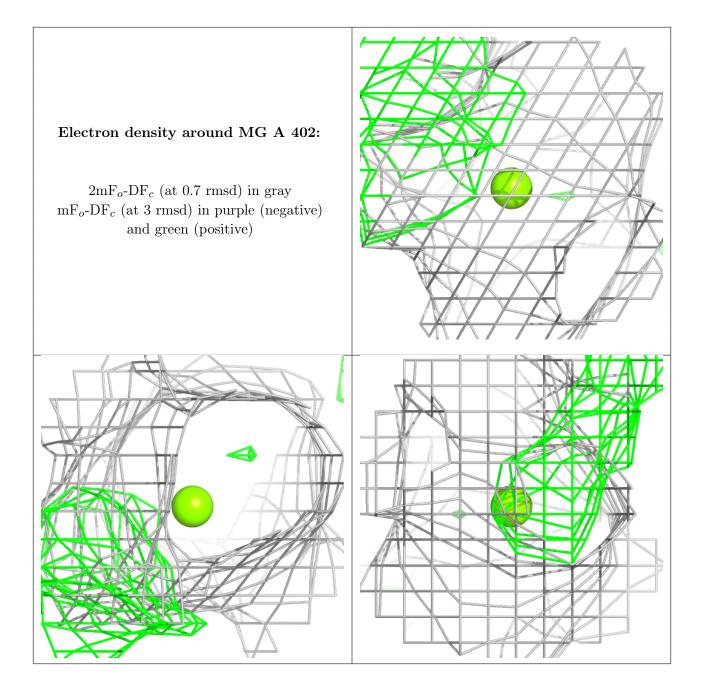




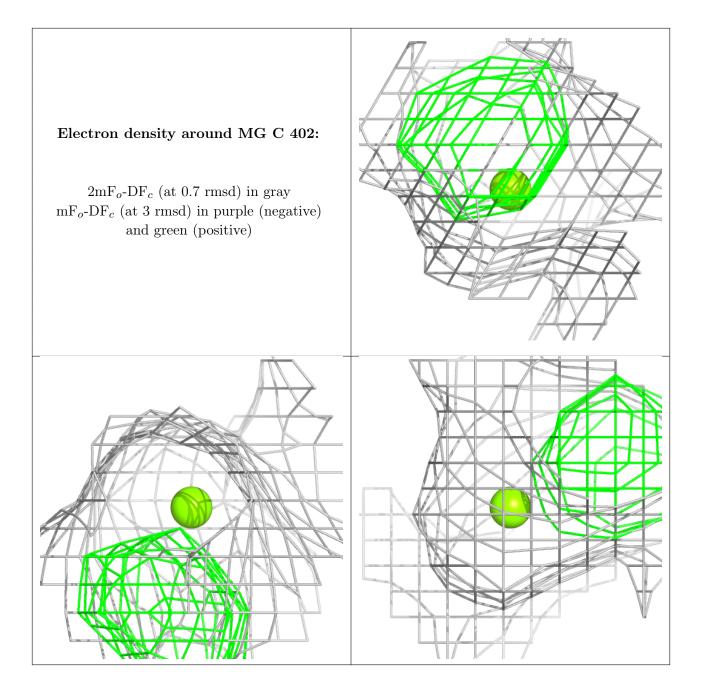




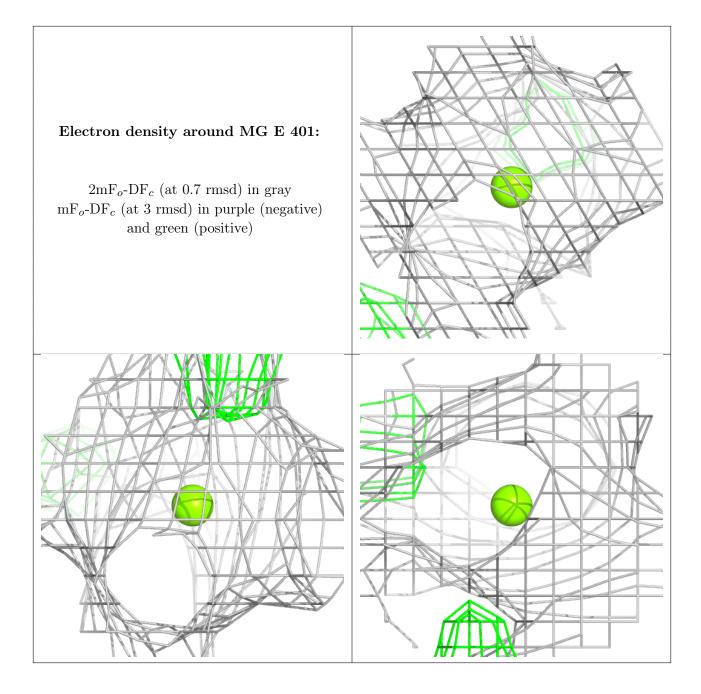




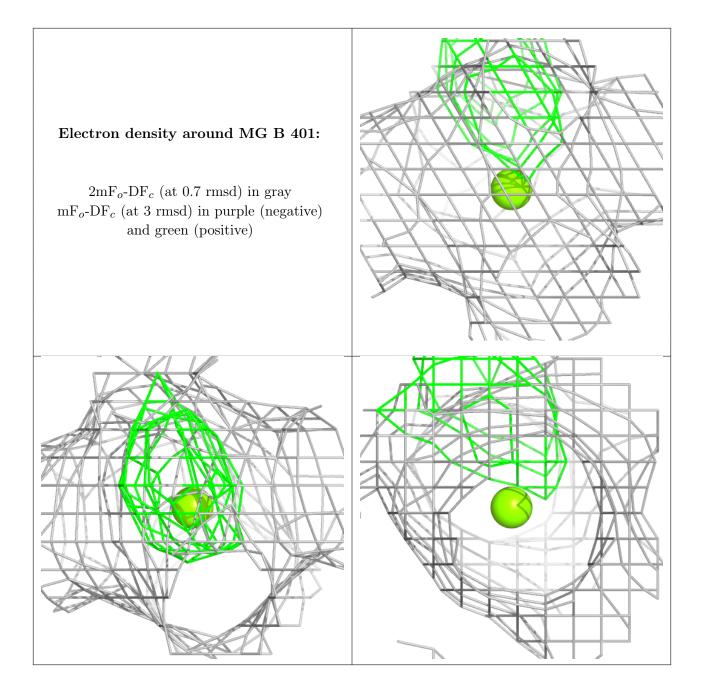




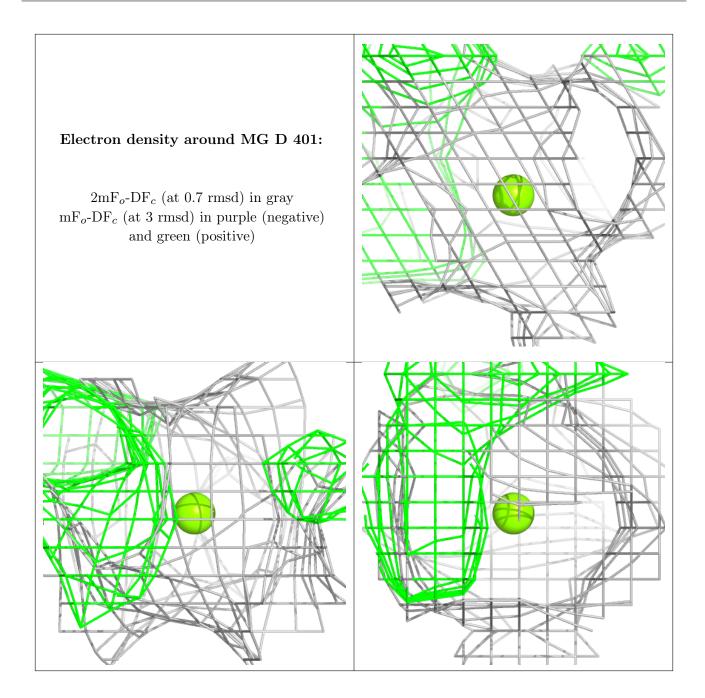












6.5 Other polymers (i)

There are no such residues in this entry.

