



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 26, 2025 – 04:10 PM EST

PDB ID : 9EJN
Title : Crystal structure of magnesium-transporting ATPase MgtA in an E1-like magnesium-bound state
Authors : Khan, M.B.; Primeau, J.O.; Basu, P.C.; Morth, J.P.; Lemieux, M.J.; Young, H.S.
Deposited on : 2024-11-28
Resolution : 3.55 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	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

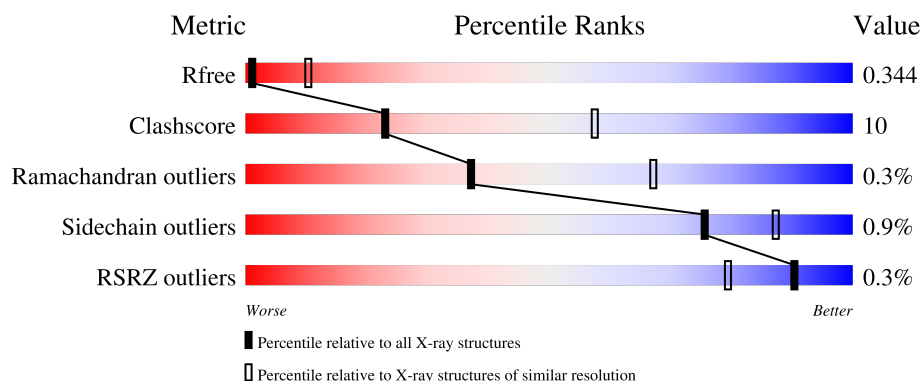
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1261 (3.62-3.50)
Clashscore	180529	1351 (3.62-3.50)
Ramachandran outliers	177936	1336 (3.62-3.50)
Sidechain outliers	177891	1337 (3.62-3.50)
RSRZ outliers	164620	1260 (3.62-3.50)

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	921	
1	B	921	
1	C	921	
1	D	921	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27352 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 Magnesium-transporting ATPase, P-type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	889	Total	C	N	O	S	0	0	0
			6837	4403	1106	1286	42			
1	C	889	Total	C	N	O	S	0	0	0
			6837	4403	1106	1286	42			
1	B	889	Total	C	N	O	S	0	0	0
			6837	4403	1106	1286	42			
1	D	889	Total	C	N	O	S	0	0	0
			6837	4403	1106	1286	42			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP A0A1V0NGB6
A	-9	HIS	-	expression tag	UNP A0A1V0NGB6
A	-8	HIS	-	expression tag	UNP A0A1V0NGB6
A	-7	HIS	-	expression tag	UNP A0A1V0NGB6
A	-6	HIS	-	expression tag	UNP A0A1V0NGB6
A	-5	HIS	-	expression tag	UNP A0A1V0NGB6
A	-4	HIS	-	expression tag	UNP A0A1V0NGB6
A	-3	HIS	-	expression tag	UNP A0A1V0NGB6
A	-2	HIS	-	expression tag	UNP A0A1V0NGB6
A	-1	LEU	-	expression tag	UNP A0A1V0NGB6
A	0	GLU	-	expression tag	UNP A0A1V0NGB6
A	216	ALA	ASP	conflict	UNP A0A1V0NGB6
A	217	ALA	GLU	conflict	UNP A0A1V0NGB6
A	218	ALA	LYS	conflict	UNP A0A1V0NGB6
A	219	ALA	ASP	conflict	UNP A0A1V0NGB6
A	220	ALA	ASP	conflict	UNP A0A1V0NGB6
A	603	ALA	LYS	conflict	UNP A0A1V0NGB6
A	606	ALA	LYS	conflict	UNP A0A1V0NGB6
A	607	ALA	GLU	conflict	UNP A0A1V0NGB6
C	-10	MET	-	initiating methionine	UNP A0A1V0NGB6
C	-9	HIS	-	expression tag	UNP A0A1V0NGB6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	HIS	-	expression tag	UNP A0A1V0NGB6
C	-7	HIS	-	expression tag	UNP A0A1V0NGB6
C	-6	HIS	-	expression tag	UNP A0A1V0NGB6
C	-5	HIS	-	expression tag	UNP A0A1V0NGB6
C	-4	HIS	-	expression tag	UNP A0A1V0NGB6
C	-3	HIS	-	expression tag	UNP A0A1V0NGB6
C	-2	HIS	-	expression tag	UNP A0A1V0NGB6
C	-1	LEU	-	expression tag	UNP A0A1V0NGB6
C	0	GLU	-	expression tag	UNP A0A1V0NGB6
C	216	ALA	ASP	conflict	UNP A0A1V0NGB6
C	217	ALA	GLU	conflict	UNP A0A1V0NGB6
C	218	ALA	LYS	conflict	UNP A0A1V0NGB6
C	219	ALA	ASP	conflict	UNP A0A1V0NGB6
C	220	ALA	ASP	conflict	UNP A0A1V0NGB6
C	603	ALA	LYS	conflict	UNP A0A1V0NGB6
C	606	ALA	LYS	conflict	UNP A0A1V0NGB6
C	607	ALA	GLU	conflict	UNP A0A1V0NGB6
B	-10	MET	-	initiating methionine	UNP A0A1V0NGB6
B	-9	HIS	-	expression tag	UNP A0A1V0NGB6
B	-8	HIS	-	expression tag	UNP A0A1V0NGB6
B	-7	HIS	-	expression tag	UNP A0A1V0NGB6
B	-6	HIS	-	expression tag	UNP A0A1V0NGB6
B	-5	HIS	-	expression tag	UNP A0A1V0NGB6
B	-4	HIS	-	expression tag	UNP A0A1V0NGB6
B	-3	HIS	-	expression tag	UNP A0A1V0NGB6
B	-2	HIS	-	expression tag	UNP A0A1V0NGB6
B	-1	LEU	-	expression tag	UNP A0A1V0NGB6
B	0	GLU	-	expression tag	UNP A0A1V0NGB6
B	216	ALA	ASP	conflict	UNP A0A1V0NGB6
B	217	ALA	GLU	conflict	UNP A0A1V0NGB6
B	218	ALA	LYS	conflict	UNP A0A1V0NGB6
B	219	ALA	ASP	conflict	UNP A0A1V0NGB6
B	220	ALA	ASP	conflict	UNP A0A1V0NGB6
B	603	ALA	LYS	conflict	UNP A0A1V0NGB6
B	606	ALA	LYS	conflict	UNP A0A1V0NGB6
B	607	ALA	GLU	conflict	UNP A0A1V0NGB6
D	-10	MET	-	initiating methionine	UNP A0A1V0NGB6
D	-9	HIS	-	expression tag	UNP A0A1V0NGB6
D	-8	HIS	-	expression tag	UNP A0A1V0NGB6
D	-7	HIS	-	expression tag	UNP A0A1V0NGB6
D	-6	HIS	-	expression tag	UNP A0A1V0NGB6
D	-5	HIS	-	expression tag	UNP A0A1V0NGB6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	-	expression tag	UNP A0A1V0NGB6
D	-3	HIS	-	expression tag	UNP A0A1V0NGB6
D	-2	HIS	-	expression tag	UNP A0A1V0NGB6
D	-1	LEU	-	expression tag	UNP A0A1V0NGB6
D	0	GLU	-	expression tag	UNP A0A1V0NGB6
D	216	ALA	ASP	conflict	UNP A0A1V0NGB6
D	217	ALA	GLU	conflict	UNP A0A1V0NGB6
D	218	ALA	LYS	conflict	UNP A0A1V0NGB6
D	219	ALA	ASP	conflict	UNP A0A1V0NGB6
D	220	ALA	ASP	conflict	UNP A0A1V0NGB6
D	603	ALA	LYS	conflict	UNP A0A1V0NGB6
D	606	ALA	LYS	conflict	UNP A0A1V0NGB6
D	607	ALA	GLU	conflict	UNP A0A1V0NGB6

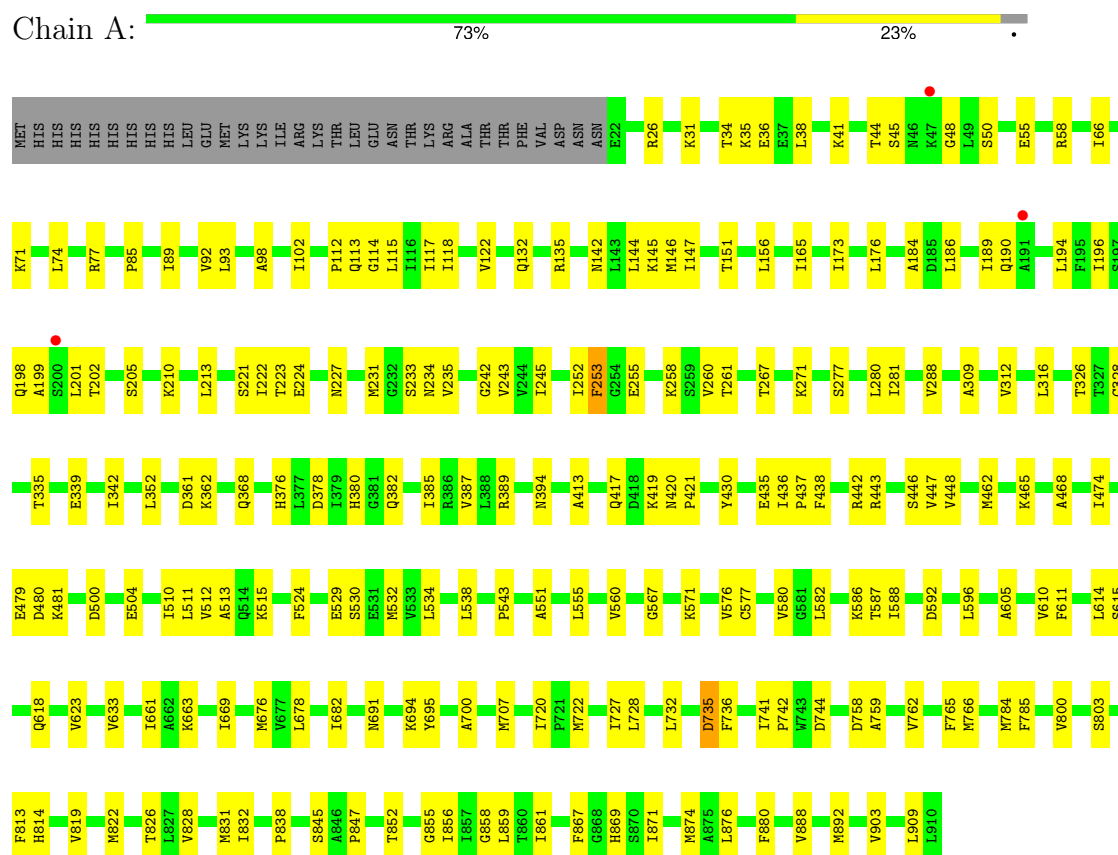
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

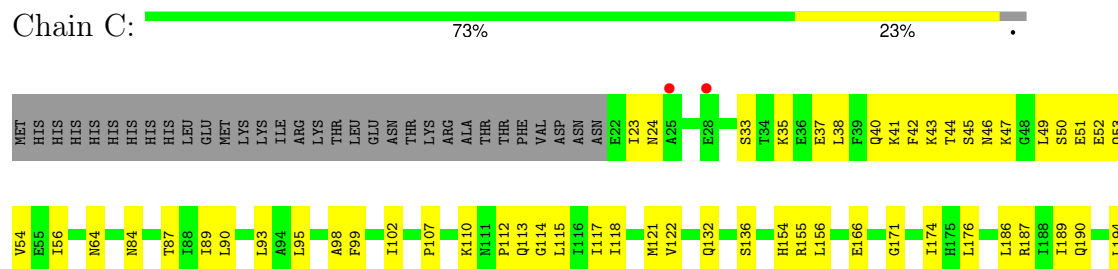
3 Residue-property plots

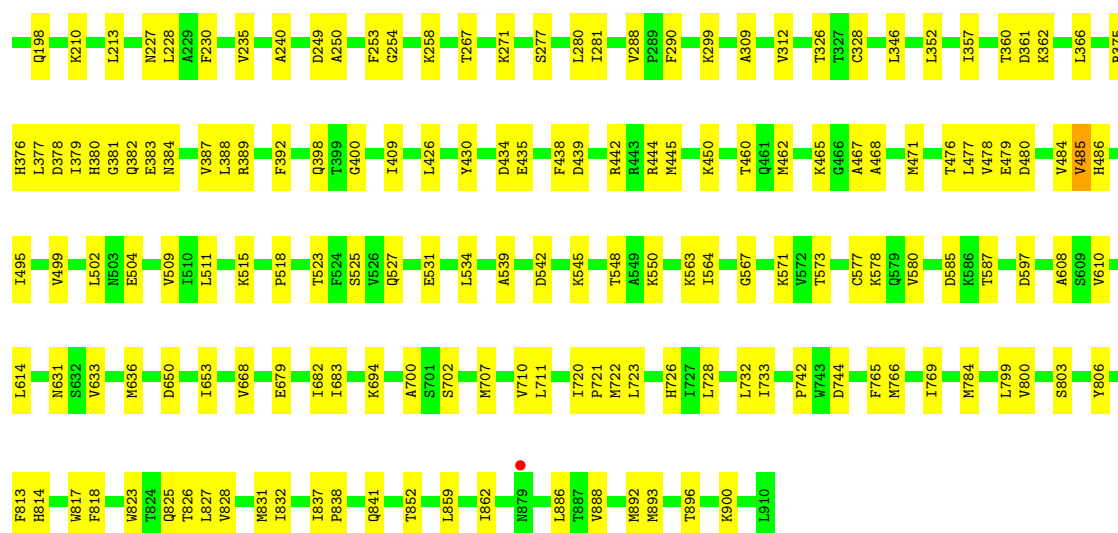
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Magnesium-transporting ATPase, P-type 1



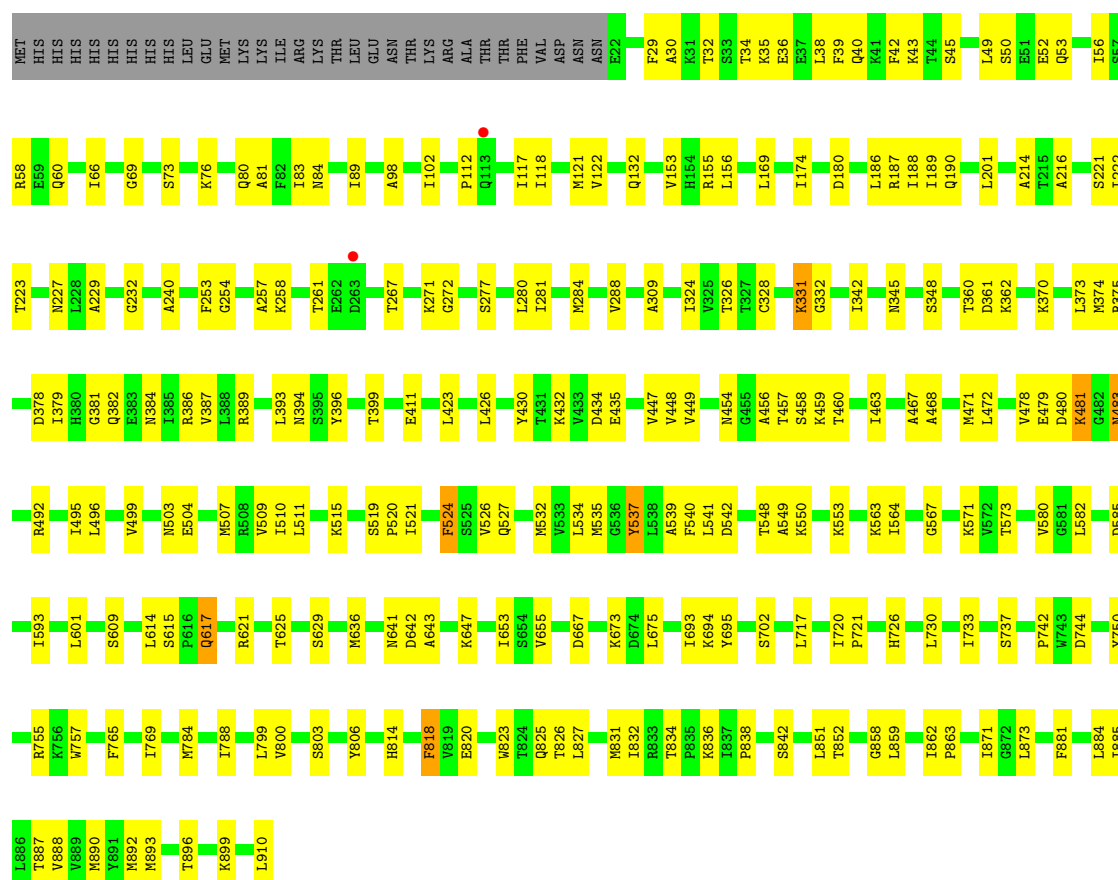
- Molecule 1: Magnesium-transporting ATPase, P-type 1





• Molecule 1: Magnesium-transporting ATPase, P-type 1

Chain B: 71% 25%



• Molecule 1: Magnesium-transporting ATPase, P-type 1

Chain D: 72% 25%

D744	V752	W757	D758	A759	S760	S761	L799	Y806	H814	E820	S821	H822	Q825	T826	L827	W828	I829	I832	R833	T834	S842	I856	L859	P863	F867	I871	G872	L873	F881	W882	L884	I885	L886	T887	W888	M892	M893	K899	L910						
V610	F611	L614	S615	P616	Q617	Q618	I622	T625	A513	L626	R627	Y635	N641	M646	S649	L827	I829	D874	L675	Y689	A690	N691	K694	Y695	I696	K697	S702	L711	I720	L723	I726	I727	L728	L729	L730	W731	L732	I733	Y734	D735	I741	P742	W743		
I495	V499	L502	M507	R508	W509	I510	L511	V512	Q513	Q514	K515	T516	M517	P520	I521	S530	M532	L538	A539	F540	L541	K545	Y558	G567	D570	K571	V572	T573	R574	V580	G581	L582	P583	T587	I593	D594	Q595	L596	D597	D598	N599	E600	L601	A605	
T363	G364	T365	L366	K370	R375	H376	L377	D378	Q382	Q383	N384	V387	L393	N394	T399	E531	M532	L426	A539	F540	L541	K545	Y558	G567	D570	K571	V572	T573	R574	V580	G581	L582	P583	T587	I593	D594	Q595	L596	D597	D598	N599	E600	L601	A605	
F195	I196	S197	Q198	D212	L213	A214	S221	I222	T223	N227	V235	I236	S237	G238	S239	A240	T241	G242	V243	V244	I245	A246	T247	F253	V260	T267	K271	S277	L280	I281	V288	P289	F290	A309	T326	T327	C328	I342	L186	R187	I188	Q350	D361	K362	
R68	G69	K70	K71	R77	F82	T89	N111	P112	Q113	I118	V122	G126	I127	L128	R129	F130	V131	Q132	G137	N142	I147	V153	H154	R155	L156	G159	S160	I165	V170	G171	I174	H175	L176	P183	A184	D185	L186	R187	I188	Q190	L194				
MET	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	LEU	GLU	MET	LYS	LYS	ILE	ARG	LYS	THR	LEU	GLU	ASN	ASN	E22	I23	R26	S33	T34	K35	E36	E37	L38	K41	F42	K43	T44	S45	N46	K47	G48	L49	S50	E51	E52	Q53	E59

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	180.40Å 66.59Å 218.67Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	24.91 – 3.55 24.91 – 3.55	Depositor EDS
% Data completeness (in resolution range)	98.5 (24.91-3.55) 98.2 (24.91-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.288 , 0.339 0.293 , 0.344	Depositor DCC
R_{free} test set	3137 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.348 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27352	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2188e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	0.25	0/6956	0.45	0/9426
1	B	0.24	0/6956	0.44	0/9426
1	C	0.25	0/6956	0.45	0/9426
1	D	0.25	0/6956	0.44	0/9426
All	All	0.25	0/27824	0.45	0/37704

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	6837	0	7054	143	0
1	B	6837	0	7054	144	0
1	C	6837	0	7054	143	0
1	D	6837	0	7054	143	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	27352	0	28216	567	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 10.

The worst 5 of 567 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:48:GLY:H	1:A:156:LEU:HD21	1.31	0.94
1:A:50:SER:H	1:A:156:LEU:HD22	1.37	0.88
1:A:210:LYS:NZ	1:A:224:GLU:O	2.14	0.79
1:A:826:THR:HG22	1:A:852:THR:HG23	1.62	0.79
1:B:331:LYS:HG2	1:B:742:PRO:HB3	1.64	0.79

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	A	887/921 (96%)	808 (91%)	77 (9%)	2 (0%)	44	74
1	B	887/921 (96%)	826 (93%)	58 (6%)	3 (0%)	37	67
1	C	887/921 (96%)	821 (93%)	62 (7%)	4 (0%)	25	59
1	D	887/921 (96%)	817 (92%)	69 (8%)	1 (0%)	48	79
All	All	3548/3684 (96%)	3272 (92%)	266 (8%)	10 (0%)	37	67

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	C	113	GLN
1	D	521	ILE
1	C	485	VAL
1	C	51	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	764/795 (96%)	758 (99%)	6 (1%)	79	89
1	B	764/795 (96%)	751 (98%)	13 (2%)	56	76
1	C	764/795 (96%)	761 (100%)	3 (0%)	89	95
1	D	764/795 (96%)	760 (100%)	4 (0%)	86	93
All	All	3056/3180 (96%)	3030 (99%)	26 (1%)	75	87

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	396	TYR
1	B	496	LEU
1	D	483	ASN
1	B	483	ASN
1	B	524	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	234	ASN
1	D	579	GLN
1	D	295	ASN
1	D	420	ASN
1	C	198	GLN

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 4 ligands modelled in this entry, 4 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	889/921 (96%)	-0.80	3 (0%) 90 79	71, 100, 144, 199	0
1	B	889/921 (96%)	-0.78	2 (0%) 92 84	73, 100, 149, 207	0
1	C	889/921 (96%)	-0.87	3 (0%) 90 79	53, 87, 144, 213	0
1	D	889/921 (96%)	-0.87	1 (0%) 92 88	51, 86, 139, 192	0
All	All	3556/3684 (96%)	-0.83	9 (0%) 90 79	51, 94, 144, 213	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	LYS	3.2
1	C	28	GLU	2.9
1	C	25	ALA	2.7
1	B	263	ASP	2.5
1	A	191	ALA	2.3

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](#)

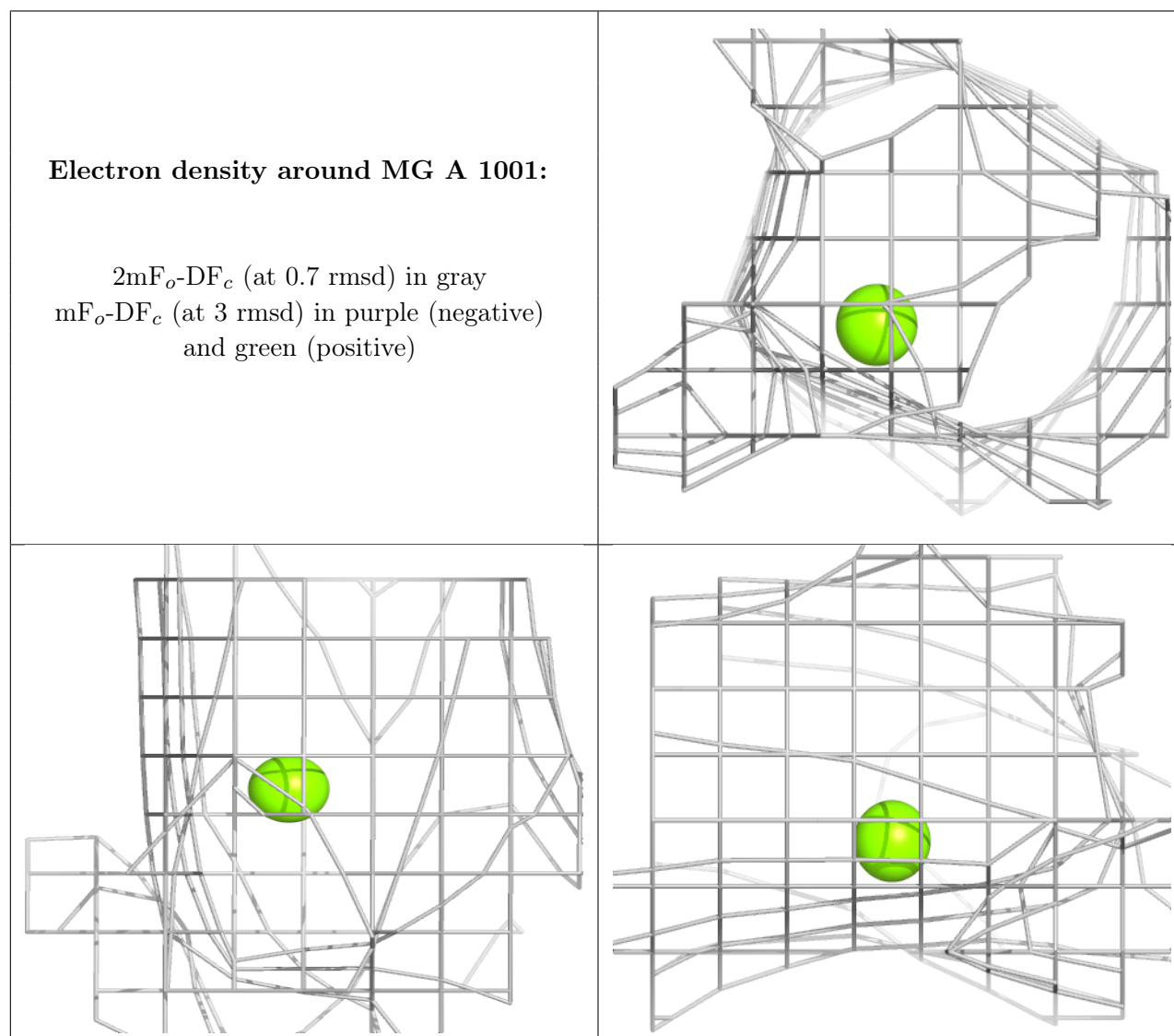
There are no monosaccharides in this entry.

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, 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.

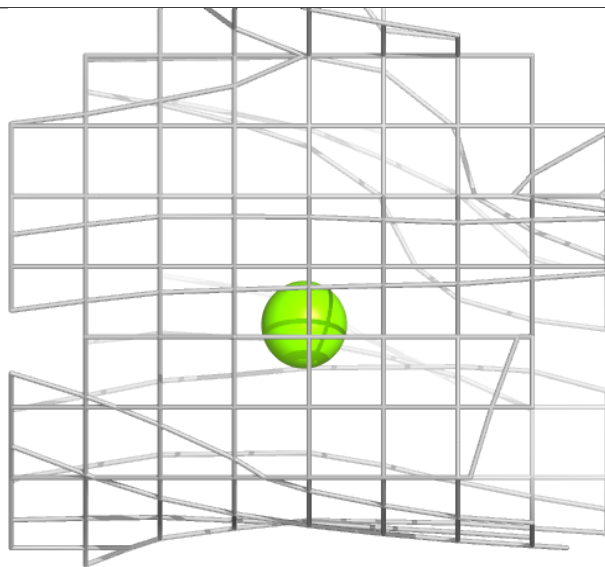
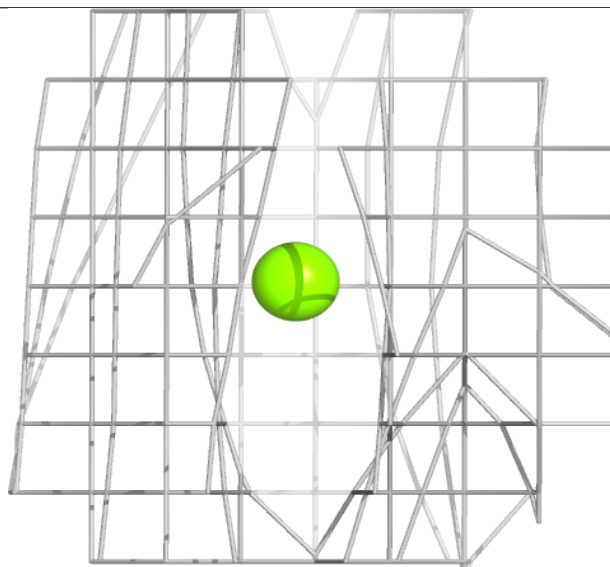
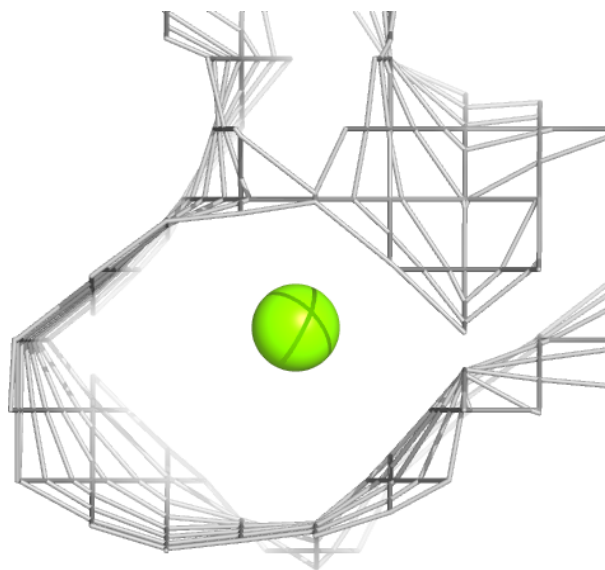
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	A	1001	1/1	0.99	0.04	78,78,78,78	0
2	MG	C	1001	1/1	0.99	0.04	61,61,61,61	0
2	MG	B	1001	1/1	0.99	0.06	75,75,75,75	0
2	MG	D	1001	1/1	1.00	0.03	53,53,53,53	0

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.



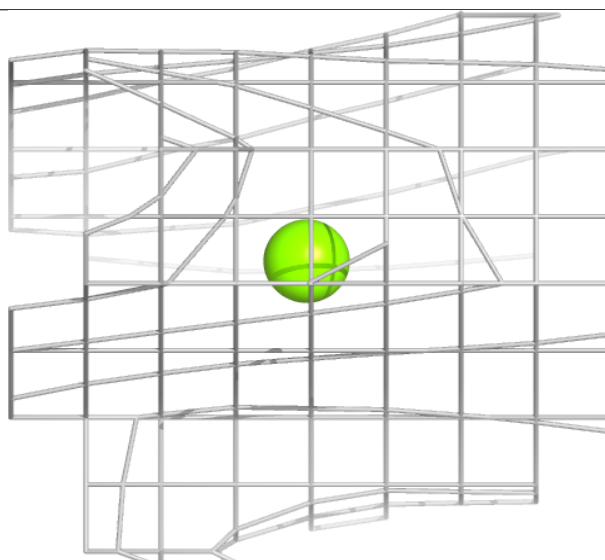
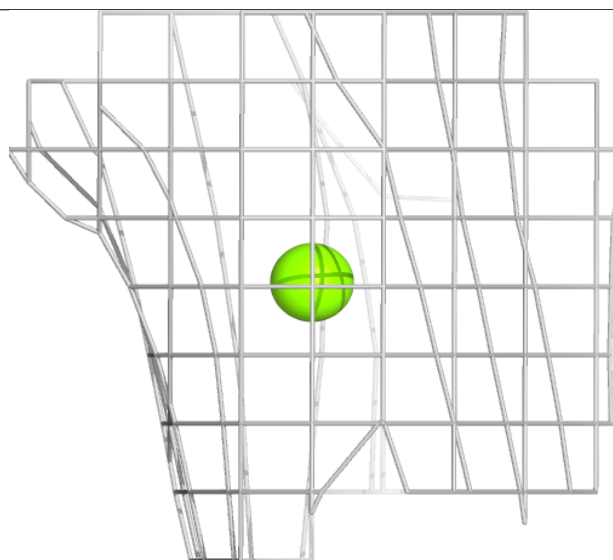
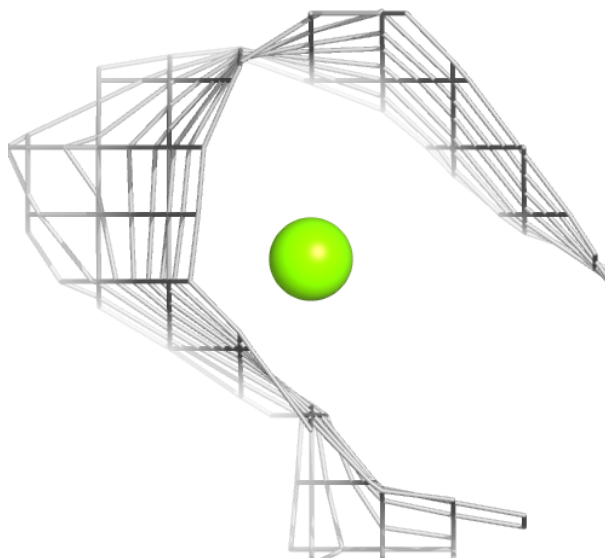
Electron density around MG C 1001:

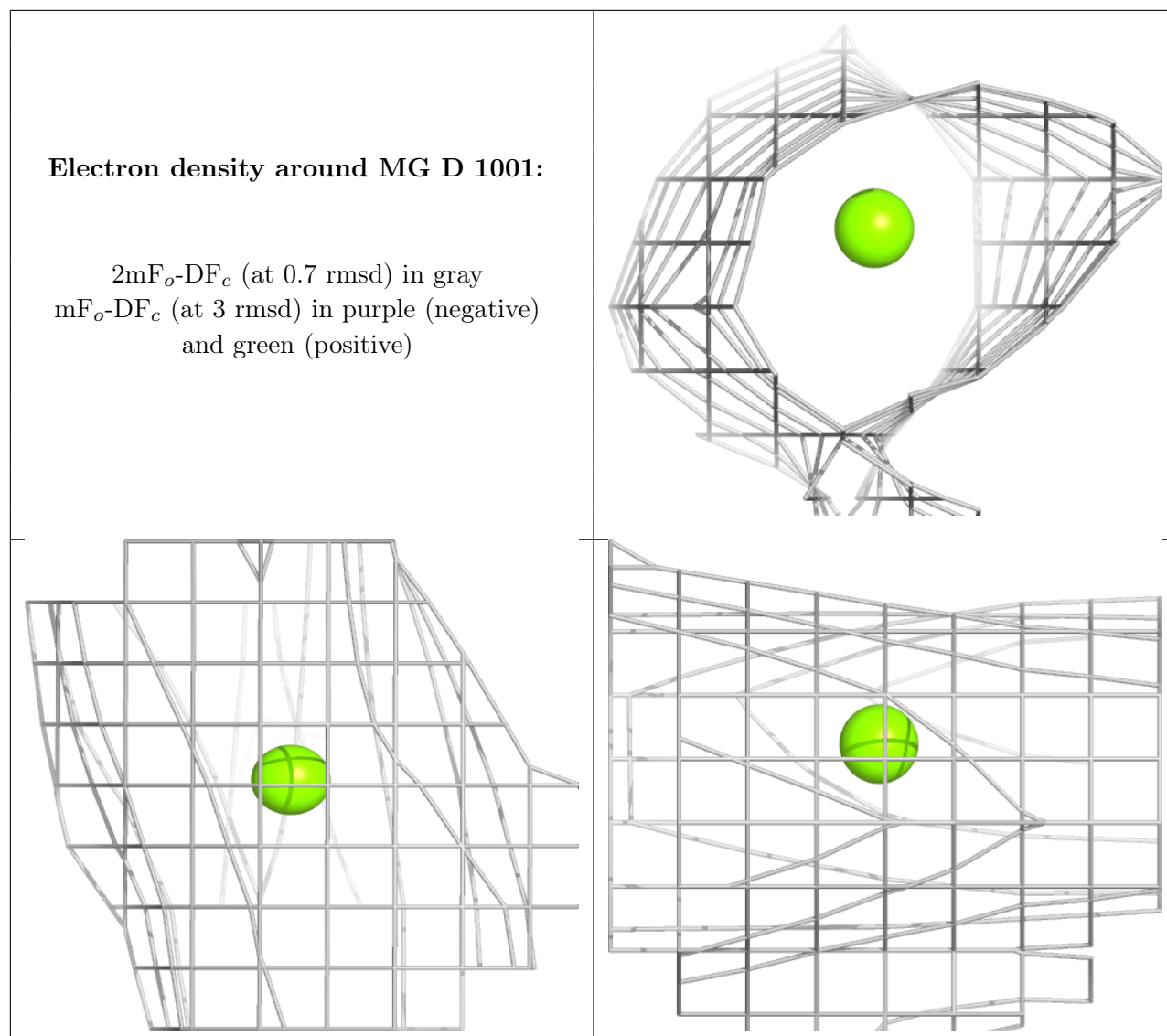
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG B 1001:

$2mF_o-DF_c$ (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.