



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:26 AM UTC

PDB ID : 9EJN / pdb_00009ejn
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	:	4-5-2 with Phenix2.0
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

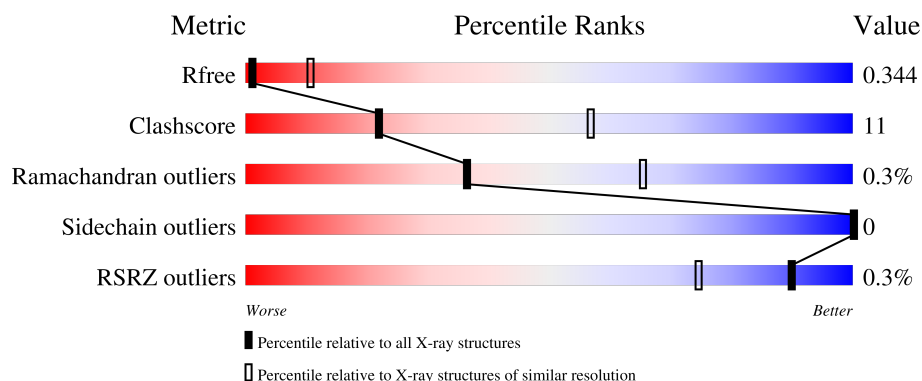
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

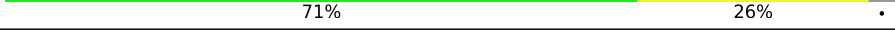
The reported resolution of this entry is 3.55 Å.

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}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

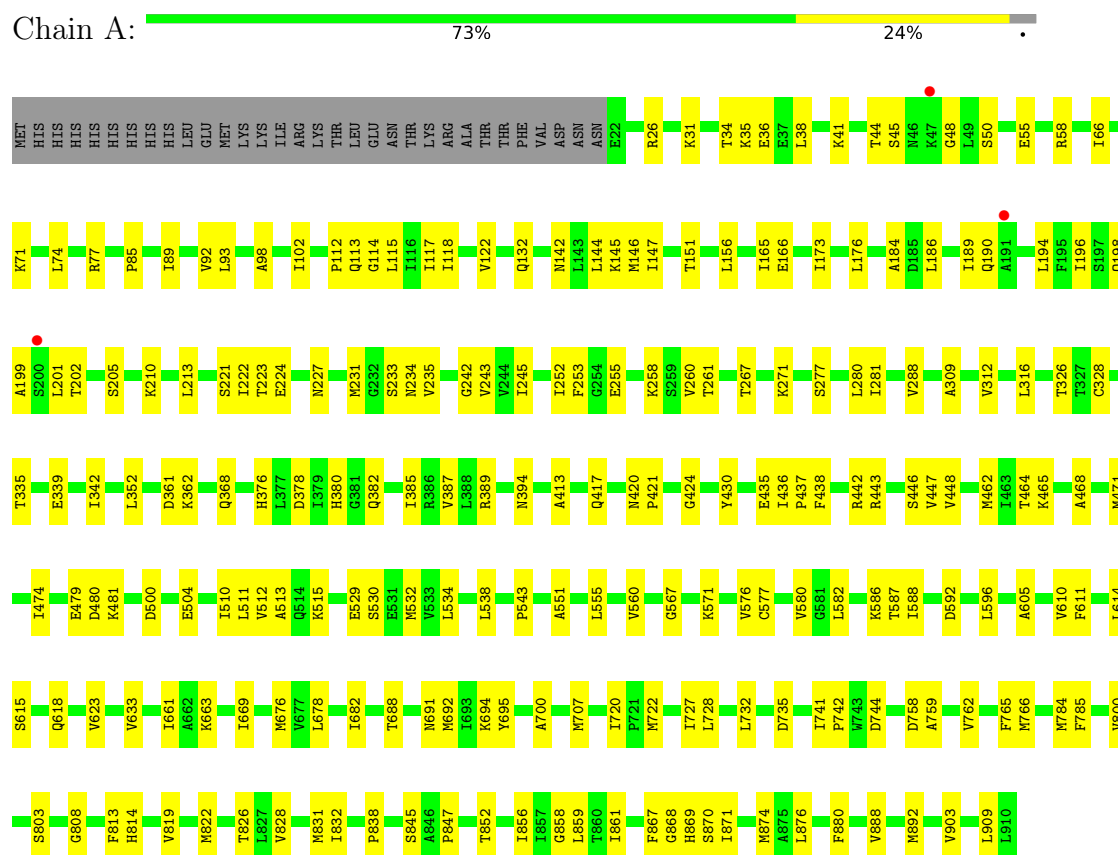
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

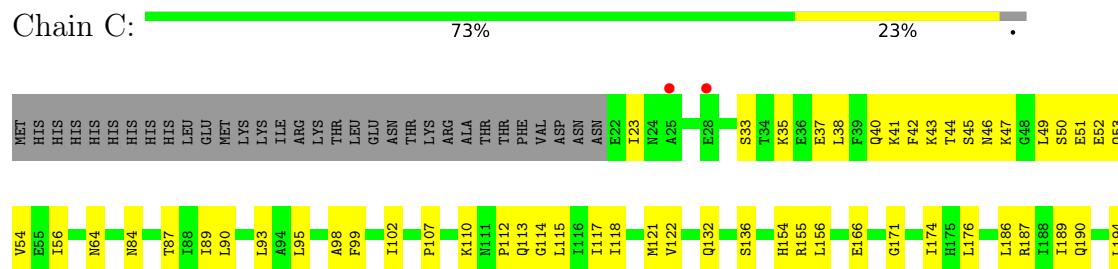
3 Residue-property plots

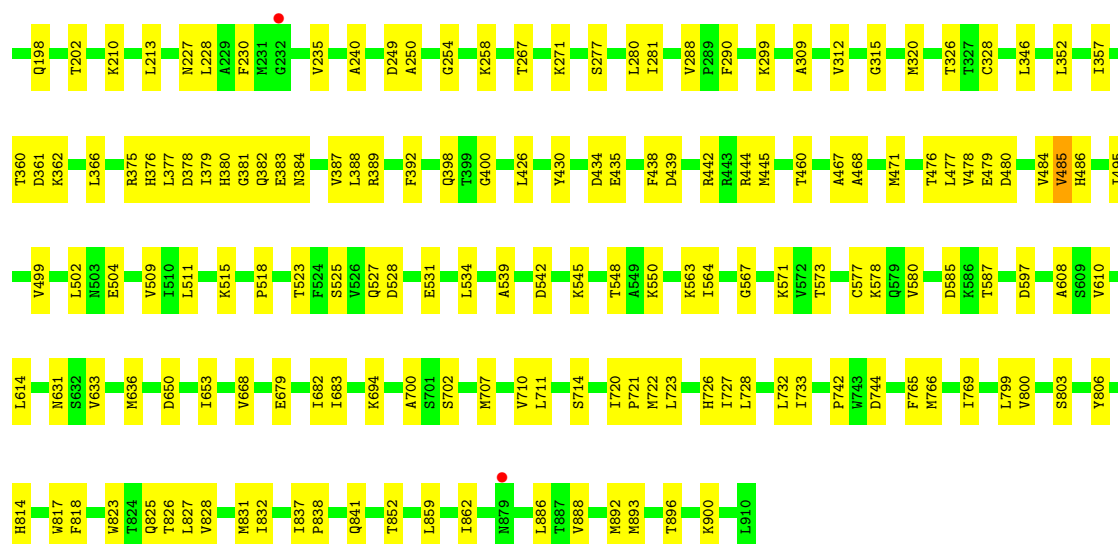
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



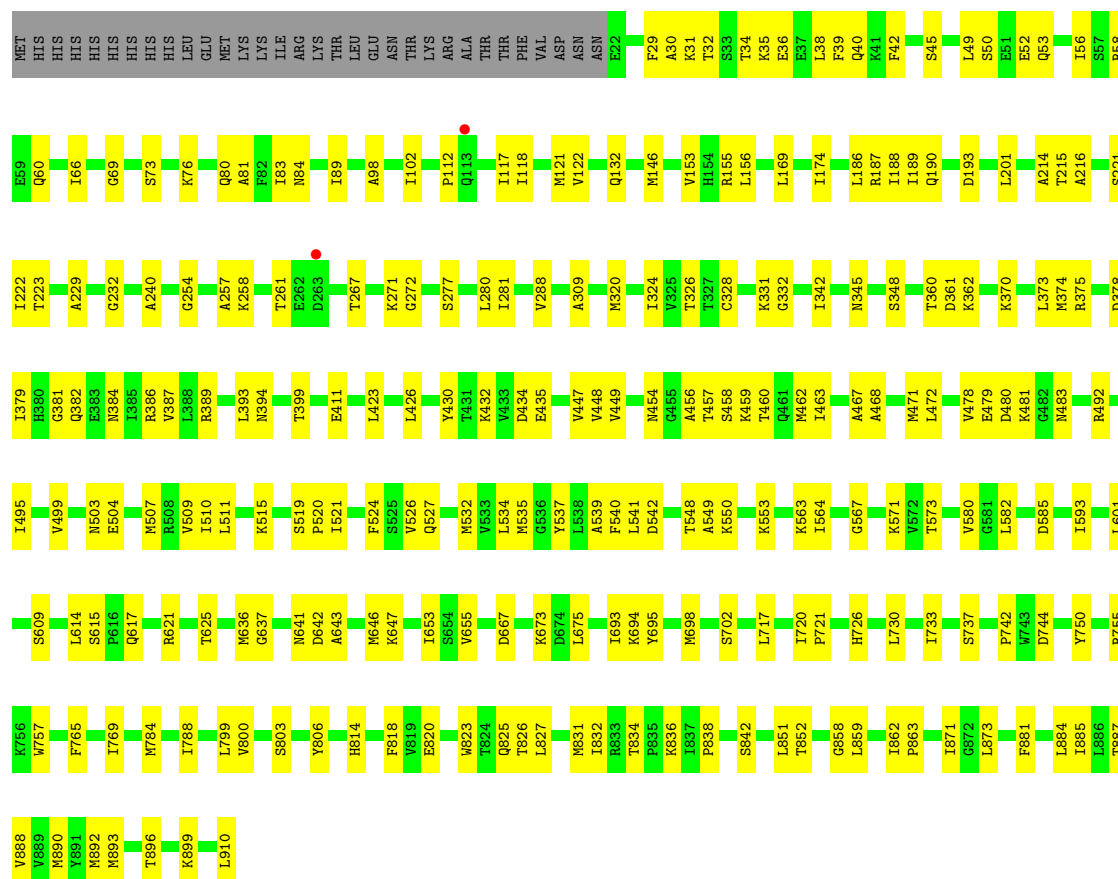
- Molecule 1: Magnesium-transporting ATPase, P-type 1





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

Chain B:  71% 26% .



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

Chain D:  71% 26% .

L884	H726	T587	T474	I342	R187	E59	MET
L885	I727	I693	C475	N345	I188	R68	HIS
L886	L728	D594	T476	N346	I189	G69	HIS
T887	L729	Q595	L477	Q350	Q190	K70	HIS
V888	L730	L596	V478	D361	L194	K71	HIS
	L731	D597	E479	K362	F195	R77	HIS
M882	L732	D598	D480	K363	I196		HIS
M893	L733	M599	V484	T363	S197	F82	HIS
	L734	E600	V484	C364	Q198		LEU
K899	D735	L601	L491	L365	T202	I89	GLU
L910				L366			MET
	I741	A605	T495	K370	D212	M11	LYS
P742	D743	V610	V499	R375	I213	Q112	LYS
D744		F611		H376	A214	Q113	ILE
	V752	L614	L502	L377	S221	I117	LYS
		S815		D378	T222	I118	THR
			M507		T223		LEU
W757	P616	Q617	R508	Q382	N227	M121	GLU
D758	Q617	Q618	V509	E383		V122	ASN
A759	D618	D618	S510	N384	G232	G126	THR
S760	S760		L511				LYS
S761		I622	V512	V387	G233	I127	ARG
			A513		V235	L128	ALA
L799		T625	Q514	L393	I236	R129	THR
		L626	K515	N394	S237	F130	THR
Y806		R627	T516		G238	V131	PHE
			N517	Q398	S239	Q132	VAL
H814		Y635			A240	G137	ASP
			P520	K419	V241		ASN
M822		N641	I521		G242	M142	ASN
			S530	L426	V243		E22
Q825		N646			V244	I147	I23
T826		S649	M532	K432	I245		R26
L827		L671		E435	A246	V153	L27
V828			L538	T436	T247	H154	E28
I829			A539	P437	V260	R155	
			F540	F438		L156	S33
			L541	D439	T267		T34
				F440		G159	K35
			K545	E441	K271	S160	E36
S842		M691		R442		I165	E37
			Y658	R443	S277		L38
T856		K694		R444			K41
		Y695	G567	N445	L280	V170	F42
L859		L696	D570	S446	I281	G171	K43
			K571	V447	V288	I174	T44
P863		K696	V572	V448	F289	H175	S45
			T573		F290	L176	N46
F867		S702	R574	Q461			K47
					A309	M181	G48
I871		L711	V580	T464		V182	L49
G872			G581	K465	T326	P183	S50
L873		I720	L582	G466	T327	A184	E51
			P583	A467	C328	D185	E52
						Q53	Q53
F881		P721				L186	
P882		L723					
W883							

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	4208 reflections (4.84%)	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 , 65.5	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.*

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

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	0.10	0/6956	0.29	0/9426
1	B	0.10	0/6956	0.26	0/9426
1	C	0.10	0/6956	0.28	0/9426
1	D	0.10	0/6956	0.28	0/9426
All	All	0.10	0/27824	0.28	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	150	0
1	B	6837	0	7054	150	0
1	C	6837	0	7054	149	0
1	D	6837	0	7054	149	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	592	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 11.

The worst 5 of 592 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%)	43	73
1	B	887/921 (96%)	826 (93%)	58 (6%)	3 (0%)	36	65
1	C	887/921 (96%)	821 (93%)	62 (7%)	4 (0%)	24	57
1	D	887/921 (96%)	817 (92%)	69 (8%)	1 (0%)	48	79
All	All	3548/3684 (96%)	3272 (92%)	266 (8%)	10 (0%)	36	65

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%)	764 (100%)	0	100	100
1	B	764/795 (96%)	764 (100%)	0	100	100
1	C	764/795 (96%)	764 (100%)	0	100	100
1	D	764/795 (96%)	764 (100%)	0	100	100
All	All	3056/3180 (96%)	3056 (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. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	138	ASN
1	B	726	HIS
1	D	726	HIS
1	B	142	ASN
1	B	503	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 oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.63	3 (0%) 90 74	71, 100, 144, 199	0
1	B	889/921 (96%)	-0.60	2 (0%) 91 80	73, 100, 149, 207	0
1	C	889/921 (96%)	-0.69	4 (0%) 88 70	53, 87, 144, 213	0
1	D	889/921 (96%)	-0.69	2 (0%) 91 80	51, 86, 139, 192	0
All	All	3556/3684 (96%)	-0.66	11 (0%) 90 74	51, 94, 144, 213	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	LYS	3.4
1	C	28	GLU	3.1
1	C	25	ALA	2.9
1	B	263	ASP	2.7
1	A	191	ALA	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](#)

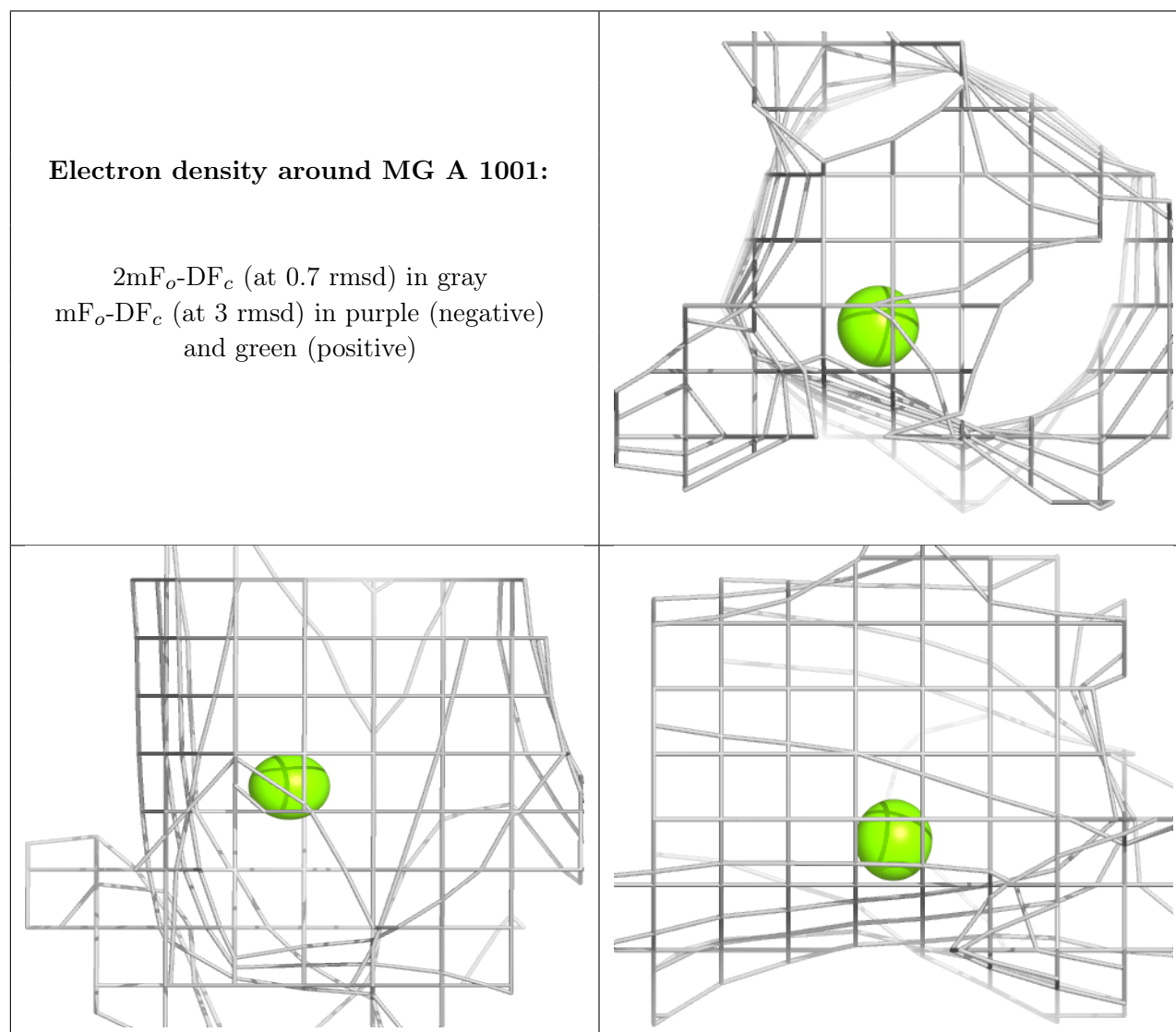
There are no oligosaccharides in this entry.

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.

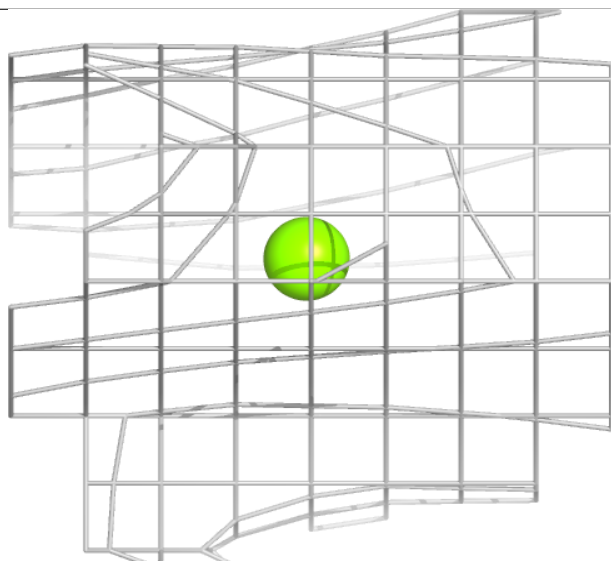
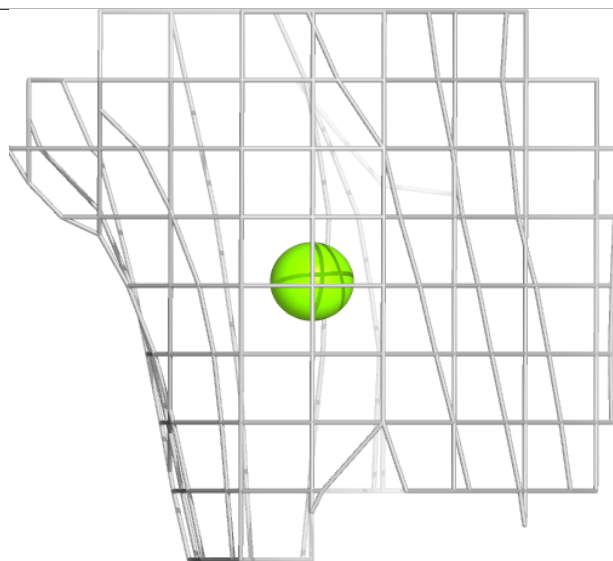
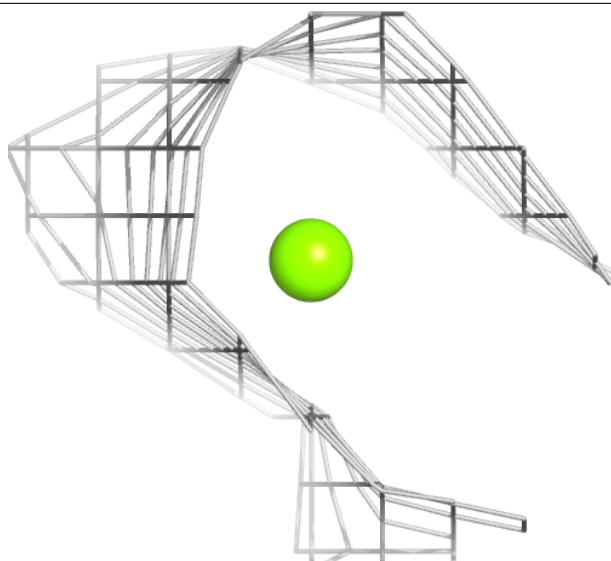
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	1001	1/1	0.99	0.04	78,78,78,78	0
2	MG	B	1001	1/1	0.99	0.06	75,75,75,75	0
2	MG	C	1001	1/1	1.00	0.03	61,61,61,61	0
2	MG	D	1001	1/1	1.00	0.03	53,53,53,53	0

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.



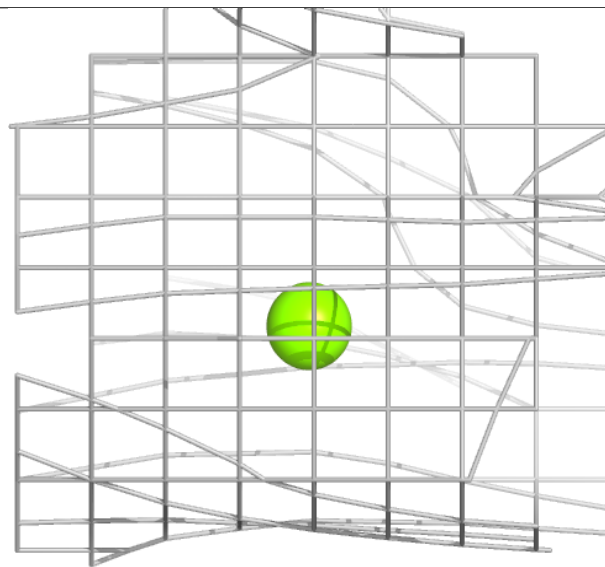
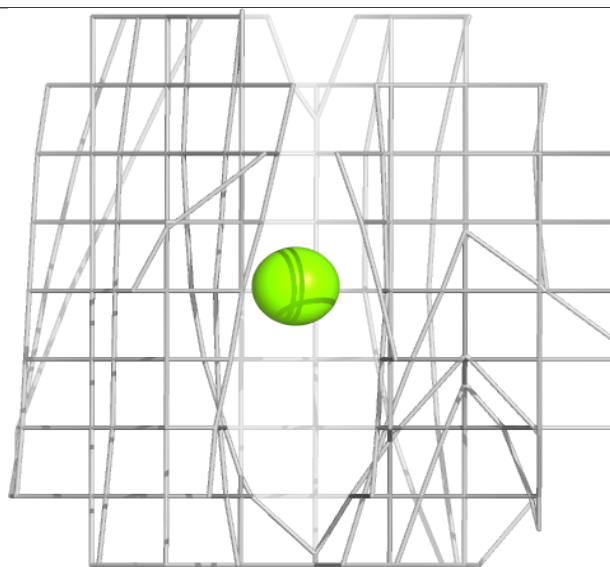
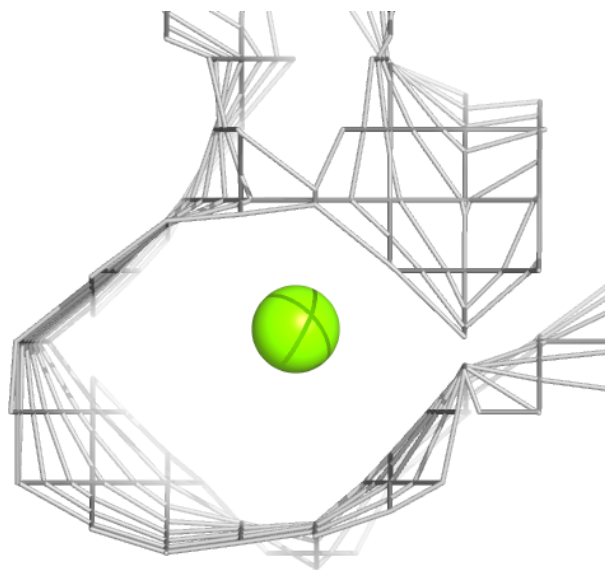
Electron density around MG B 1001:

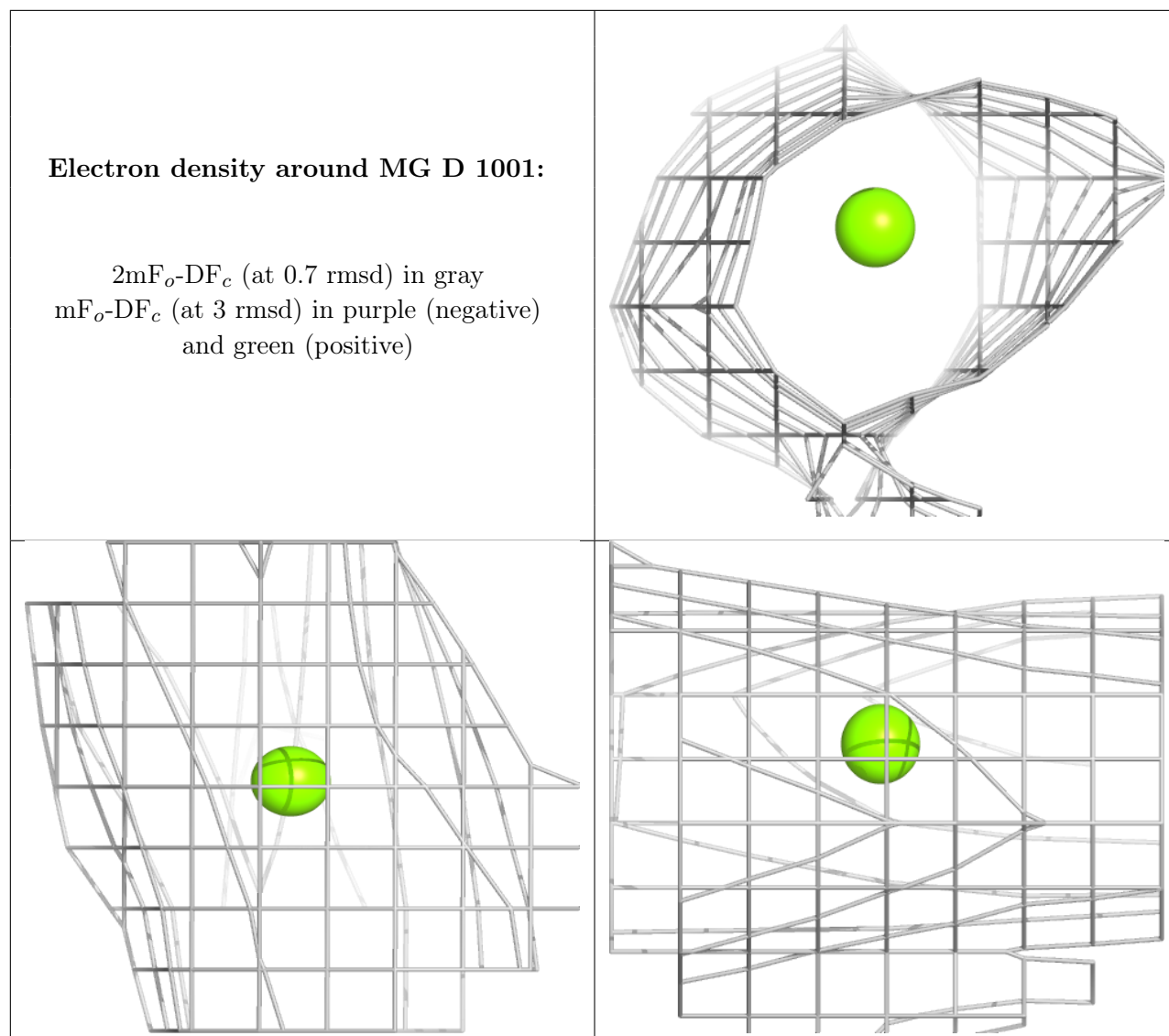
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.