



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2022 – 03:56 PM EDT

PDB ID : 7TNI
Title : Structure of EC12 Y1392W variant of BT-R1 from *Manduca sexta*, a Cry1A toxin binding domain
Authors : Fisher, A.J.; Wilcox, X.E.
Deposited on : 2022-01-21
Resolution : 1.90 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.28.1
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)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

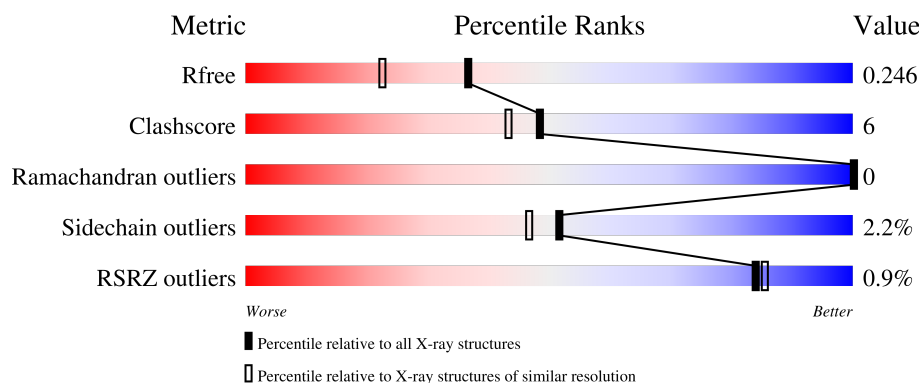
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	155	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>7%</div> <div>29%</div> </div> </div>
1	B	155	<div> <div>%</div> <div> <div></div> <div>56%</div> <div>14%</div> <div>..</div> <div>29%</div> </div> </div>
1	C	155	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>9%</div> <div>28%</div> </div> </div>
1	D	155	<div> <div></div> <div> <div>63%</div> <div>7%</div> <div>•</div> <div>29%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3651 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 Cadherin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	0	3	0
			857	538	149	168	2			
1	B	110	Total	C	N	O	S	0	3	0
			855	537	146	170	2			
1	C	111	Total	C	N	O	S	0	2	0
			857	537	146	172	2			
1	D	110	Total	C	N	O	S	0	2	0
			851	534	148	167	2			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1306	MET	-	initiating methionine	UNP Q8MZK3
A	1307	ASN	-	expression tag	UNP Q8MZK3
A	1308	THR	-	expression tag	UNP Q8MZK3
A	1309	ILE	-	expression tag	UNP Q8MZK3
A	1310	HIS	-	expression tag	UNP Q8MZK3
A	1311	HIS	-	expression tag	UNP Q8MZK3
A	1312	HIS	-	expression tag	UNP Q8MZK3
A	1313	HIS	-	expression tag	UNP Q8MZK3
A	1314	HIS	-	expression tag	UNP Q8MZK3
A	1315	HIS	-	expression tag	UNP Q8MZK3
A	1316	ASN	-	expression tag	UNP Q8MZK3
A	1317	THR	-	expression tag	UNP Q8MZK3
A	1318	SER	-	expression tag	UNP Q8MZK3
A	1319	GLY	-	expression tag	UNP Q8MZK3
A	1320	SER	-	expression tag	UNP Q8MZK3
A	1321	GLY	-	expression tag	UNP Q8MZK3
A	1322	GLY	-	expression tag	UNP Q8MZK3
A	1323	GLY	-	expression tag	UNP Q8MZK3
A	1324	GLY	-	expression tag	UNP Q8MZK3
A	1325	GLY	-	expression tag	UNP Q8MZK3
A	1326	ARG	-	expression tag	UNP Q8MZK3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1327	LEU	-	expression tag	UNP Q8MZK3
A	1328	VAL	-	expression tag	UNP Q8MZK3
A	1329	PRO	-	expression tag	UNP Q8MZK3
A	1330	ARG	-	expression tag	UNP Q8MZK3
A	1331	GLY	-	expression tag	UNP Q8MZK3
A	1332	SER	-	expression tag	UNP Q8MZK3
A	1333	MET	-	expression tag	UNP Q8MZK3
A	1334	SER	-	expression tag	UNP Q8MZK3
A	1335	GLU	-	expression tag	UNP Q8MZK3
A	1336	ASN	-	expression tag	UNP Q8MZK3
A	1337	LEU	-	expression tag	UNP Q8MZK3
A	1338	TYR	-	expression tag	UNP Q8MZK3
A	1339	PHE	-	expression tag	UNP Q8MZK3
A	1340	GLN	-	expression tag	UNP Q8MZK3
A	1341	GLY	-	expression tag	UNP Q8MZK3
A	1342	SER	-	expression tag	UNP Q8MZK3
A	1343	MET	-	expression tag	UNP Q8MZK3
A	1344	ASP	-	expression tag	UNP Q8MZK3
A	1345	ILE	-	expression tag	UNP Q8MZK3
A	1346	GLU	-	expression tag	UNP Q8MZK3
A	1347	PHE	-	expression tag	UNP Q8MZK3
A	1348	VAL	-	expression tag	UNP Q8MZK3
A	1355	VAL	MET	conflict	UNP Q8MZK3
A	1384	SER	ALA	conflict	UNP Q8MZK3
A	1392	TRP	TYR	engineered mutation	UNP Q8MZK3
B	1306	MET	-	initiating methionine	UNP Q8MZK3
B	1307	ASN	-	expression tag	UNP Q8MZK3
B	1308	THR	-	expression tag	UNP Q8MZK3
B	1309	ILE	-	expression tag	UNP Q8MZK3
B	1310	HIS	-	expression tag	UNP Q8MZK3
B	1311	HIS	-	expression tag	UNP Q8MZK3
B	1312	HIS	-	expression tag	UNP Q8MZK3
B	1313	HIS	-	expression tag	UNP Q8MZK3
B	1314	HIS	-	expression tag	UNP Q8MZK3
B	1315	HIS	-	expression tag	UNP Q8MZK3
B	1316	ASN	-	expression tag	UNP Q8MZK3
B	1317	THR	-	expression tag	UNP Q8MZK3
B	1318	SER	-	expression tag	UNP Q8MZK3
B	1319	GLY	-	expression tag	UNP Q8MZK3
B	1320	SER	-	expression tag	UNP Q8MZK3
B	1321	GLY	-	expression tag	UNP Q8MZK3
B	1322	GLY	-	expression tag	UNP Q8MZK3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1323	GLY	-	expression tag	UNP Q8MZK3
B	1324	GLY	-	expression tag	UNP Q8MZK3
B	1325	GLY	-	expression tag	UNP Q8MZK3
B	1326	ARG	-	expression tag	UNP Q8MZK3
B	1327	LEU	-	expression tag	UNP Q8MZK3
B	1328	VAL	-	expression tag	UNP Q8MZK3
B	1329	PRO	-	expression tag	UNP Q8MZK3
B	1330	ARG	-	expression tag	UNP Q8MZK3
B	1331	GLY	-	expression tag	UNP Q8MZK3
B	1332	SER	-	expression tag	UNP Q8MZK3
B	1333	MET	-	expression tag	UNP Q8MZK3
B	1334	SER	-	expression tag	UNP Q8MZK3
B	1335	GLU	-	expression tag	UNP Q8MZK3
B	1336	ASN	-	expression tag	UNP Q8MZK3
B	1337	LEU	-	expression tag	UNP Q8MZK3
B	1338	TYR	-	expression tag	UNP Q8MZK3
B	1339	PHE	-	expression tag	UNP Q8MZK3
B	1340	GLN	-	expression tag	UNP Q8MZK3
B	1341	GLY	-	expression tag	UNP Q8MZK3
B	1342	SER	-	expression tag	UNP Q8MZK3
B	1343	MET	-	expression tag	UNP Q8MZK3
B	1344	ASP	-	expression tag	UNP Q8MZK3
B	1345	ILE	-	expression tag	UNP Q8MZK3
B	1346	GLU	-	expression tag	UNP Q8MZK3
B	1347	PHE	-	expression tag	UNP Q8MZK3
B	1348	VAL	-	expression tag	UNP Q8MZK3
B	1355	VAL	MET	conflict	UNP Q8MZK3
B	1384	SER	ALA	conflict	UNP Q8MZK3
B	1392	TRP	TYR	engineered mutation	UNP Q8MZK3
C	1306	MET	-	initiating methionine	UNP Q8MZK3
C	1307	ASN	-	expression tag	UNP Q8MZK3
C	1308	THR	-	expression tag	UNP Q8MZK3
C	1309	ILE	-	expression tag	UNP Q8MZK3
C	1310	HIS	-	expression tag	UNP Q8MZK3
C	1311	HIS	-	expression tag	UNP Q8MZK3
C	1312	HIS	-	expression tag	UNP Q8MZK3
C	1313	HIS	-	expression tag	UNP Q8MZK3
C	1314	HIS	-	expression tag	UNP Q8MZK3
C	1315	HIS	-	expression tag	UNP Q8MZK3
C	1316	ASN	-	expression tag	UNP Q8MZK3
C	1317	THR	-	expression tag	UNP Q8MZK3
C	1318	SER	-	expression tag	UNP Q8MZK3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1319	GLY	-	expression tag	UNP Q8MZK3
C	1320	SER	-	expression tag	UNP Q8MZK3
C	1321	GLY	-	expression tag	UNP Q8MZK3
C	1322	GLY	-	expression tag	UNP Q8MZK3
C	1323	GLY	-	expression tag	UNP Q8MZK3
C	1324	GLY	-	expression tag	UNP Q8MZK3
C	1325	GLY	-	expression tag	UNP Q8MZK3
C	1326	ARG	-	expression tag	UNP Q8MZK3
C	1327	LEU	-	expression tag	UNP Q8MZK3
C	1328	VAL	-	expression tag	UNP Q8MZK3
C	1329	PRO	-	expression tag	UNP Q8MZK3
C	1330	ARG	-	expression tag	UNP Q8MZK3
C	1331	GLY	-	expression tag	UNP Q8MZK3
C	1332	SER	-	expression tag	UNP Q8MZK3
C	1333	MET	-	expression tag	UNP Q8MZK3
C	1334	SER	-	expression tag	UNP Q8MZK3
C	1335	GLU	-	expression tag	UNP Q8MZK3
C	1336	ASN	-	expression tag	UNP Q8MZK3
C	1337	LEU	-	expression tag	UNP Q8MZK3
C	1338	TYR	-	expression tag	UNP Q8MZK3
C	1339	PHE	-	expression tag	UNP Q8MZK3
C	1340	GLN	-	expression tag	UNP Q8MZK3
C	1341	GLY	-	expression tag	UNP Q8MZK3
C	1342	SER	-	expression tag	UNP Q8MZK3
C	1343	MET	-	expression tag	UNP Q8MZK3
C	1344	ASP	-	expression tag	UNP Q8MZK3
C	1345	ILE	-	expression tag	UNP Q8MZK3
C	1346	GLU	-	expression tag	UNP Q8MZK3
C	1347	PHE	-	expression tag	UNP Q8MZK3
C	1348	VAL	-	expression tag	UNP Q8MZK3
C	1355	VAL	MET	conflict	UNP Q8MZK3
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D	1306	MET	-	initiating methionine	UNP Q8MZK3
D	1307	ASN	-	expression tag	UNP Q8MZK3
D	1308	THR	-	expression tag	UNP Q8MZK3
D	1309	ILE	-	expression tag	UNP Q8MZK3
D	1310	HIS	-	expression tag	UNP Q8MZK3
D	1311	HIS	-	expression tag	UNP Q8MZK3
D	1312	HIS	-	expression tag	UNP Q8MZK3
D	1313	HIS	-	expression tag	UNP Q8MZK3
D	1314	HIS	-	expression tag	UNP Q8MZK3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1315	HIS	-	expression tag	UNP Q8MZK3
D	1316	ASN	-	expression tag	UNP Q8MZK3
D	1317	THR	-	expression tag	UNP Q8MZK3
D	1318	SER	-	expression tag	UNP Q8MZK3
D	1319	GLY	-	expression tag	UNP Q8MZK3
D	1320	SER	-	expression tag	UNP Q8MZK3
D	1321	GLY	-	expression tag	UNP Q8MZK3
D	1322	GLY	-	expression tag	UNP Q8MZK3
D	1323	GLY	-	expression tag	UNP Q8MZK3
D	1324	GLY	-	expression tag	UNP Q8MZK3
D	1325	GLY	-	expression tag	UNP Q8MZK3
D	1326	ARG	-	expression tag	UNP Q8MZK3
D	1327	LEU	-	expression tag	UNP Q8MZK3
D	1328	VAL	-	expression tag	UNP Q8MZK3
D	1329	PRO	-	expression tag	UNP Q8MZK3
D	1330	ARG	-	expression tag	UNP Q8MZK3
D	1331	GLY	-	expression tag	UNP Q8MZK3
D	1332	SER	-	expression tag	UNP Q8MZK3
D	1333	MET	-	expression tag	UNP Q8MZK3
D	1334	SER	-	expression tag	UNP Q8MZK3
D	1335	GLU	-	expression tag	UNP Q8MZK3
D	1336	ASN	-	expression tag	UNP Q8MZK3
D	1337	LEU	-	expression tag	UNP Q8MZK3
D	1338	TYR	-	expression tag	UNP Q8MZK3
D	1339	PHE	-	expression tag	UNP Q8MZK3
D	1340	GLN	-	expression tag	UNP Q8MZK3
D	1341	GLY	-	expression tag	UNP Q8MZK3
D	1342	SER	-	expression tag	UNP Q8MZK3
D	1343	MET	-	expression tag	UNP Q8MZK3
D	1344	ASP	-	expression tag	UNP Q8MZK3
D	1345	ILE	-	expression tag	UNP Q8MZK3
D	1346	GLU	-	expression tag	UNP Q8MZK3
D	1347	PHE	-	expression tag	UNP Q8MZK3
D	1348	VAL	-	expression tag	UNP Q8MZK3
D	1355	VAL	MET	conflict	UNP Q8MZK3
D	1384	SER	ALA	conflict	UNP Q8MZK3
D	1392	TRP	TYR	engineered mutation	UNP Q8MZK3

- 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 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0

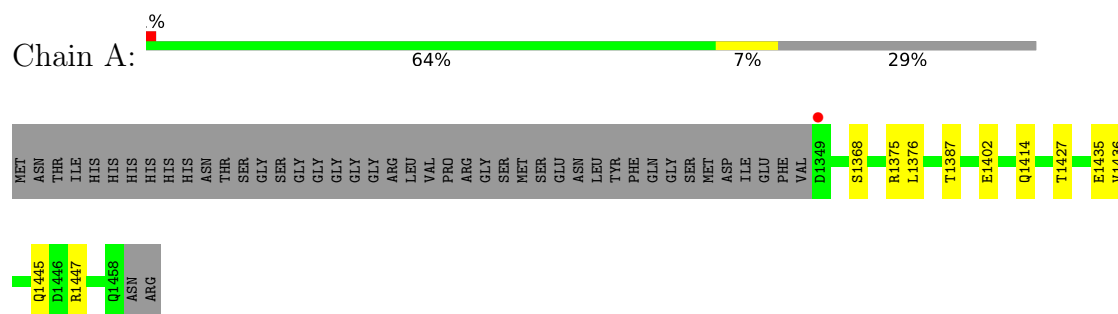
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total 40	O 40	0	0
3	B	50	Total 50	O 50	0	0
3	C	73	Total 73	O 73	0	0
3	D	64	Total 64	O 64	0	0

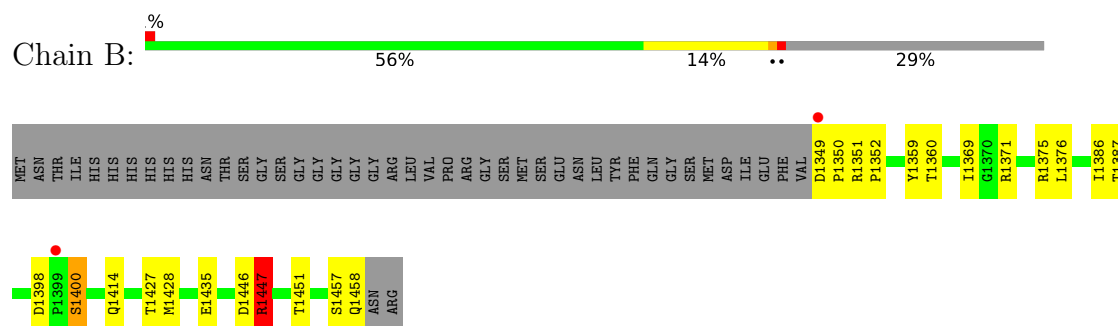
3 Residue-property plots [i](#)

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.

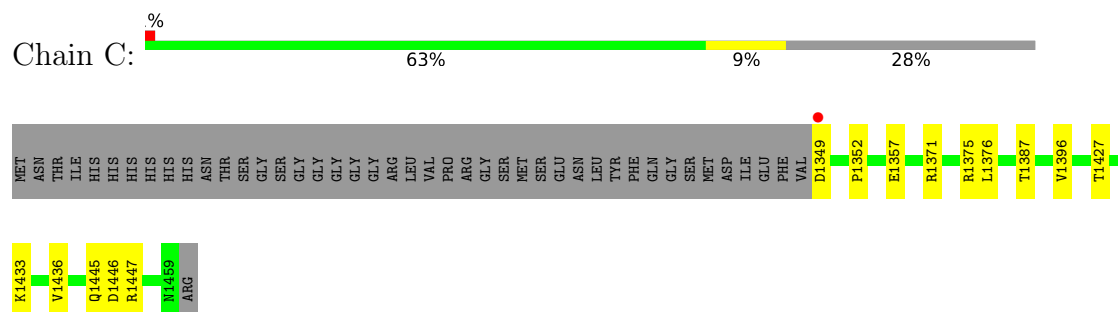
- Molecule 1: Cadherin



- Molecule 1: Cadherin

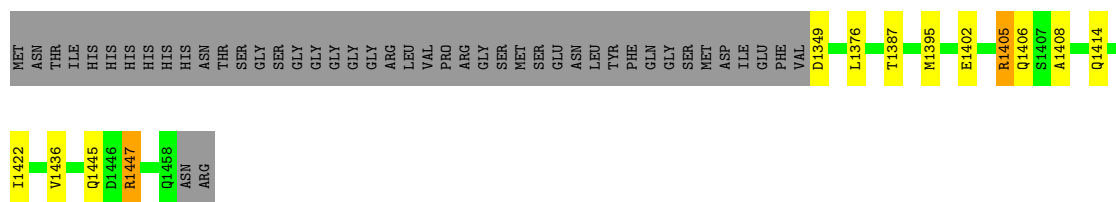


- Molecule 1: Cadherin



- Molecule 1: Cadherin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.13Å 44.58Å 94.80Å 90.00° 107.16° 90.00°	Depositor
Resolution (Å)	56.50 – 1.90 56.50 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (56.50-1.90) 99.3 (56.50-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.210 , 0.240 0.220 , 0.246	Depositor DCC
R_{free} test set	1926 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3651	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 69.29 % 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 3.7908e-06. 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

5.1 Standard geometry

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	0.83	0/880	1.00	0/1201
1	B	0.79	0/878	1.02	4/1199 (0.3%)
1	C	0.85	0/877	0.91	1/1198 (0.1%)
1	D	0.86	0/871	1.03	2/1189 (0.2%)
All	All	0.84	0/3506	0.99	7/4787 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1447[A]	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	D	1447[B]	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	B	1447	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	B	1371	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	1371	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	1375[A]	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	B	1375[B]	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	A	857	0	855	7	0
1	B	855	0	848	19	0
1	C	857	0	844	10	0
1	D	851	0	847	10	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
3	A	40	0	0	2	0
3	B	50	0	0	4	0
3	C	73	0	0	2	0
3	D	64	0	0	1	0
All	All	3651	0	3394	41	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 6.

All (41) 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:1387:THR:HG21	1:B:1387:THR:HG21	1.55	0.88
1:B:1414[B]:GLN:HG2	1:D:1414:GLN:OE1	1.75	0.87
1:C:1387:THR:HG21	1:D:1387:THR:HG21	1.57	0.86
1:A:1435:GLU:OE2	3:A:1601:HOH:O	1.96	0.82
1:C:1445:GLN:OE1	1:C:1447[B]:ARG:NH2	2.17	0.77
1:B:1414[B]:GLN:HG2	3:B:1604:HOH:O	1.90	0.71
1:C:1427:THR:OG1	3:C:1601:HOH:O	2.08	0.70
1:B:1369:ILE:O	3:B:1601:HOH:O	2.11	0.69
1:B:1351:ARG:O	3:B:1602:HOH:O	2.12	0.66
1:A:1376:LEU:HD13	1:A:1436:VAL:HG11	1.79	0.65
1:D:1445:GLN:OE1	1:D:1447[B]:ARG:NH2	2.31	0.64
3:C:1637:HOH:O	1:D:1414:GLN:HB2	1.99	0.61
1:B:1435:GLU:OE1	1:B:1447:ARG:HD3	2.03	0.59
1:B:1351:ARG:HB2	1:B:1352:PRO:HD2	1.86	0.57
1:C:1357[B]:GLU:H	1:C:1357[B]:GLU:CD	2.07	0.56
1:D:1408:ALA:HA	1:D:1422:ILE:HG12	1.89	0.55
1:D:1395:MET:O	1:D:1405[A]:ARG:NH2	2.40	0.54
1:B:1398:ASP:OD2	1:B:1400:SER:HB3	2.06	0.53
1:C:1396:VAL:HG22	1:C:1433:LYS:HB2	1.92	0.51
1:B:1414[B]:GLN:NE2	1:B:1414[B]:GLN:HA	2.26	0.51
1:B:1414[B]:GLN:HA	1:B:1414[B]:GLN:HE21	1.76	0.50
1:A:1375[A]:ARG:HD3	1:C:1375:ARG:HH21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:GLN:OE1	1:A:1447[B]:ARG:NH2	2.45	0.49
1:B:1428:MET:O	3:B:1603:HOH:O	2.20	0.49
1:C:1376:LEU:CD1	1:C:1436:VAL:HG11	2.43	0.49
1:D:1349:ASP:O	3:D:1601:HOH:O	2.20	0.49
1:A:1402:GLU:OE1	1:A:1402:GLU:HA	2.13	0.47
1:B:1349:ASP:N	1:B:1350:PRO:HD2	2.30	0.47
1:B:1359:TYR:CD1	1:B:1376:LEU:HD23	2.50	0.47
1:C:1352:PRO:O	1:C:1446:ASP:HB2	2.15	0.47
1:B:1400:SER:OG	1:B:1428:MET:HA	2.15	0.46
1:B:1352:PRO:O	1:B:1446:ASP:HB2	2.17	0.45
1:C:1387:THR:HG21	1:D:1387:THR:CG2	2.40	0.45
1:D:1376:LEU:HD13	1:D:1436:VAL:HG11	1.98	0.45
1:D:1405[A]:ARG:HG2	1:D:1406:GLN:HG2	1.98	0.44
1:B:1360:THR:HA	1:B:1451:THR:O	2.18	0.44
1:A:1414[A]:GLN:NE2	3:A:1602:HOH:O	2.47	0.44
1:B:1359:TYR:CE1	1:B:1376:LEU:HD23	2.54	0.43
1:B:1352:PRO:HB3	1:B:1386:ILE:HD12	2.01	0.43
1:C:1376:LEU:HD12	1:C:1436:VAL:HG11	2.02	0.42
1:B:1457:SER:O	1:B:1458:GLN:HB3	2.19	0.41

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	111/155 (72%)	110 (99%)	1 (1%)	0	100	100
1	B	111/155 (72%)	109 (98%)	2 (2%)	0	100	100
1	C	111/155 (72%)	110 (99%)	1 (1%)	0	100	100
1	D	110/155 (71%)	109 (99%)	1 (1%)	0	100	100
All	All	443/620 (72%)	438 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	94/129 (73%)	92 (98%)	2 (2%)	53	48
1	B	94/129 (73%)	91 (97%)	3 (3%)	39	30
1	C	94/129 (73%)	93 (99%)	1 (1%)	73	73
1	D	93/129 (72%)	90 (97%)	3 (3%)	39	30
All	All	375/516 (73%)	366 (98%)	9 (2%)	52	43

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1368	SER
1	A	1427	THR
1	B	1400	SER
1	B	1427	THR
1	B	1447	ARG
1	C	1349	ASP
1	D	1402	GLU
1	D	1405[A]	ARG
1	D	1405[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1458	GLN

5.3.3 RNA ⓘ

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 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	110/155 (70%)	-0.03	1 (0%) 84 85	33, 48, 73, 98	0
1	B	110/155 (70%)	0.22	2 (1%) 68 71	33, 50, 81, 108	0
1	C	111/155 (71%)	-0.16	1 (0%) 84 85	30, 43, 66, 101	0
1	D	110/155 (70%)	-0.24	0 100 100	30, 40, 63, 80	0
All	All	441/620 (71%)	-0.05	4 (0%) 84 85	30, 44, 74, 108	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1349	ASP	6.1
1	B	1399	PRO	3.6
1	C	1349	ASP	3.4
1	A	1349	ASP	3.0

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](#)

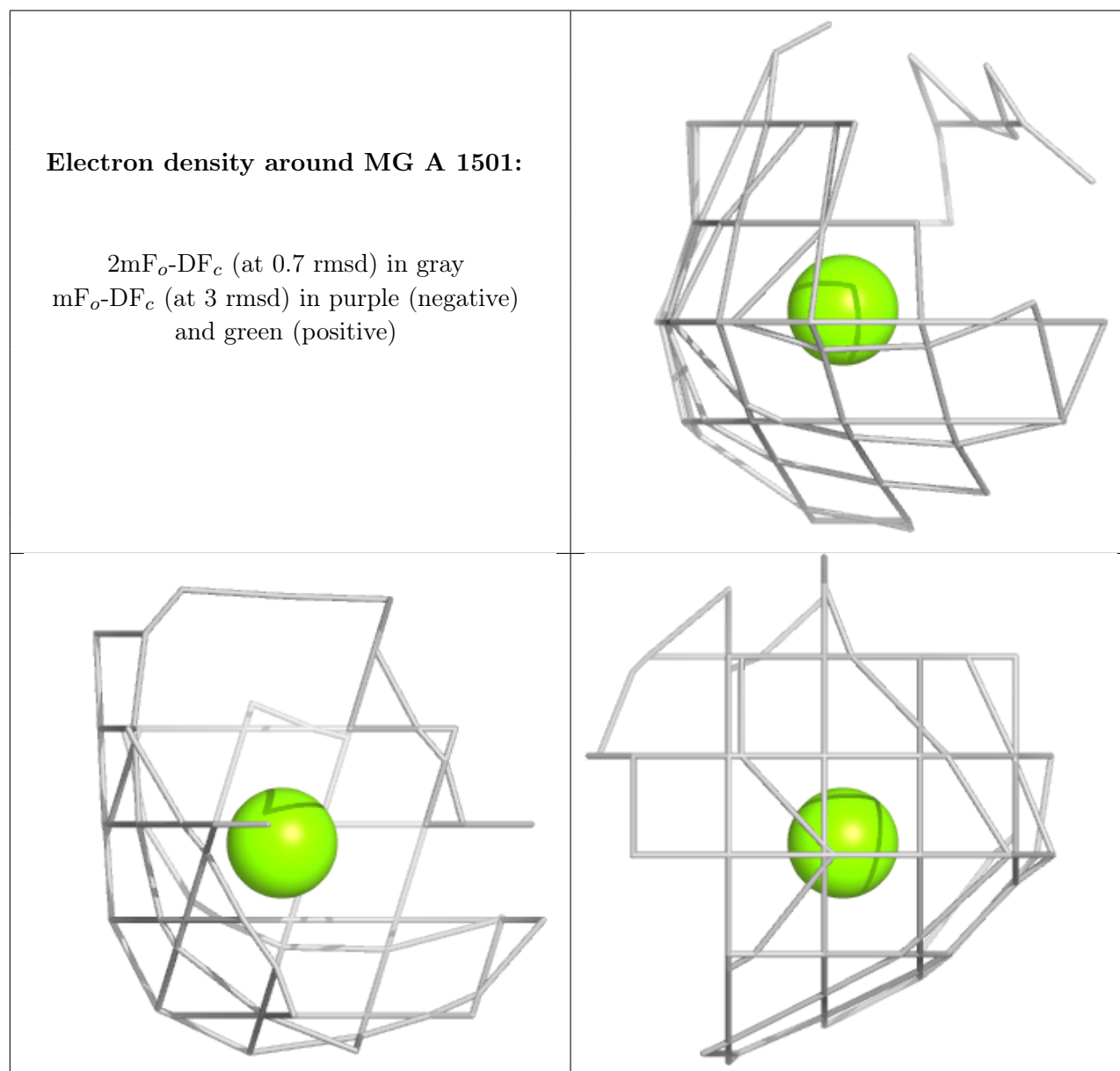
There are no monosaccharides in this entry.

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, 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.

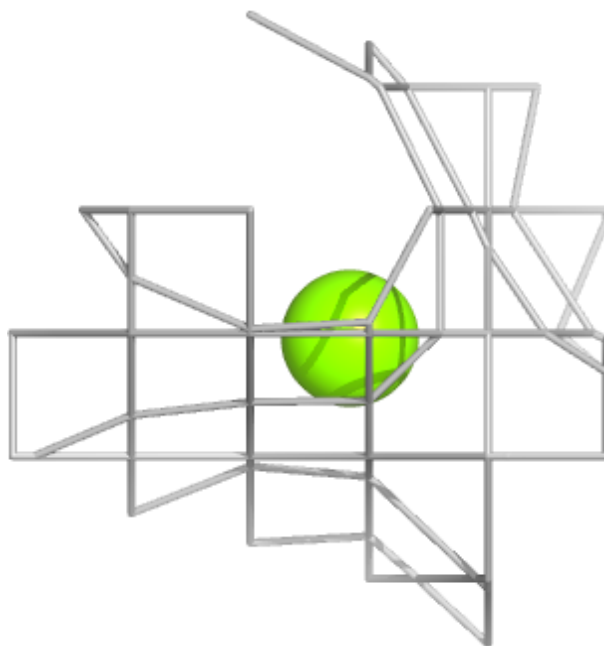
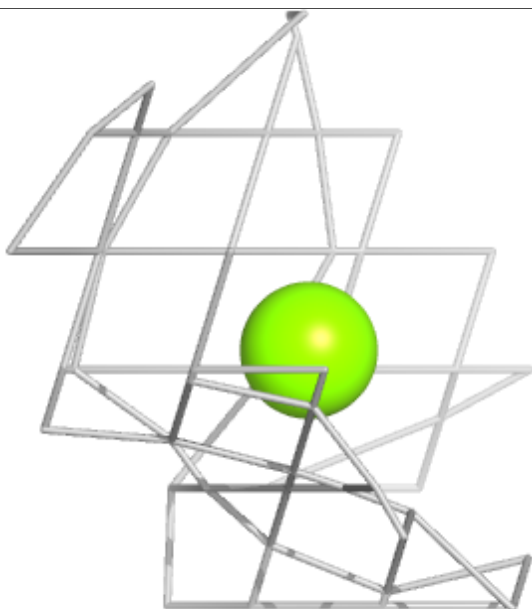
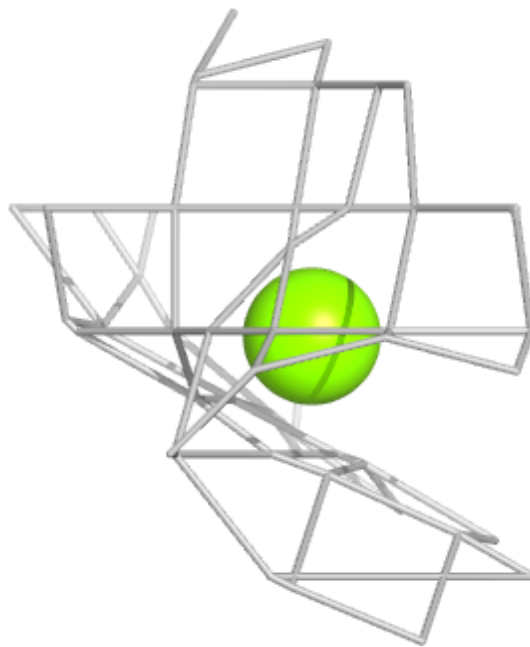
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	$Q < 0.9$
2	MG	A	1501	1/1	0.66	0.08	68,68,68,68	0
2	MG	B	1501	1/1	0.76	0.16	85,85,85,85	0
2	MG	D	1501	1/1	0.79	0.06	60,60,60,60	0
2	MG	C	1501	1/1	0.97	0.07	52,52,52,52	0

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.



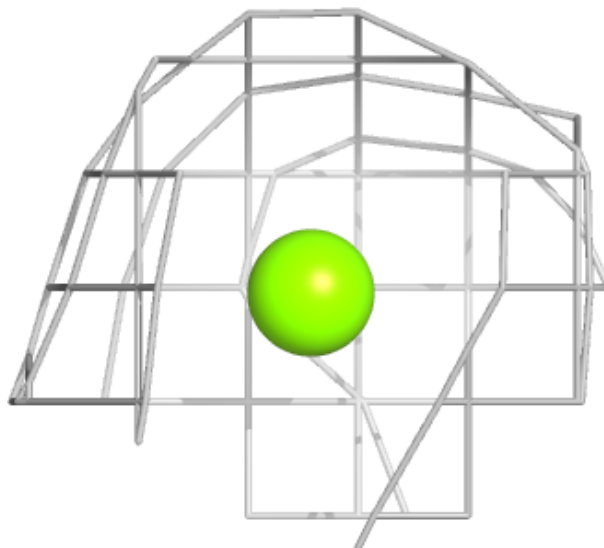
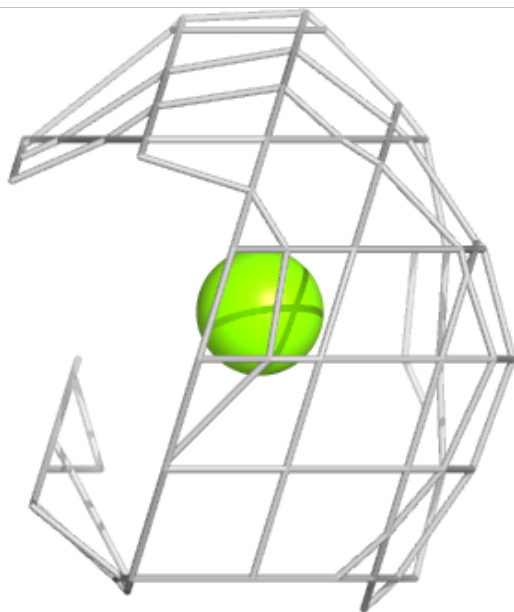
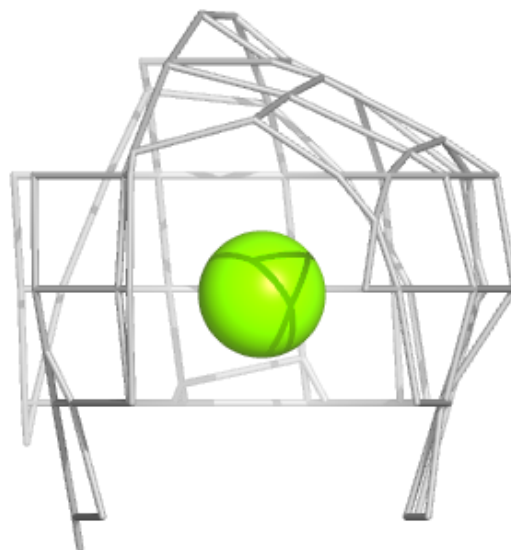
Electron density around MG B 1501:

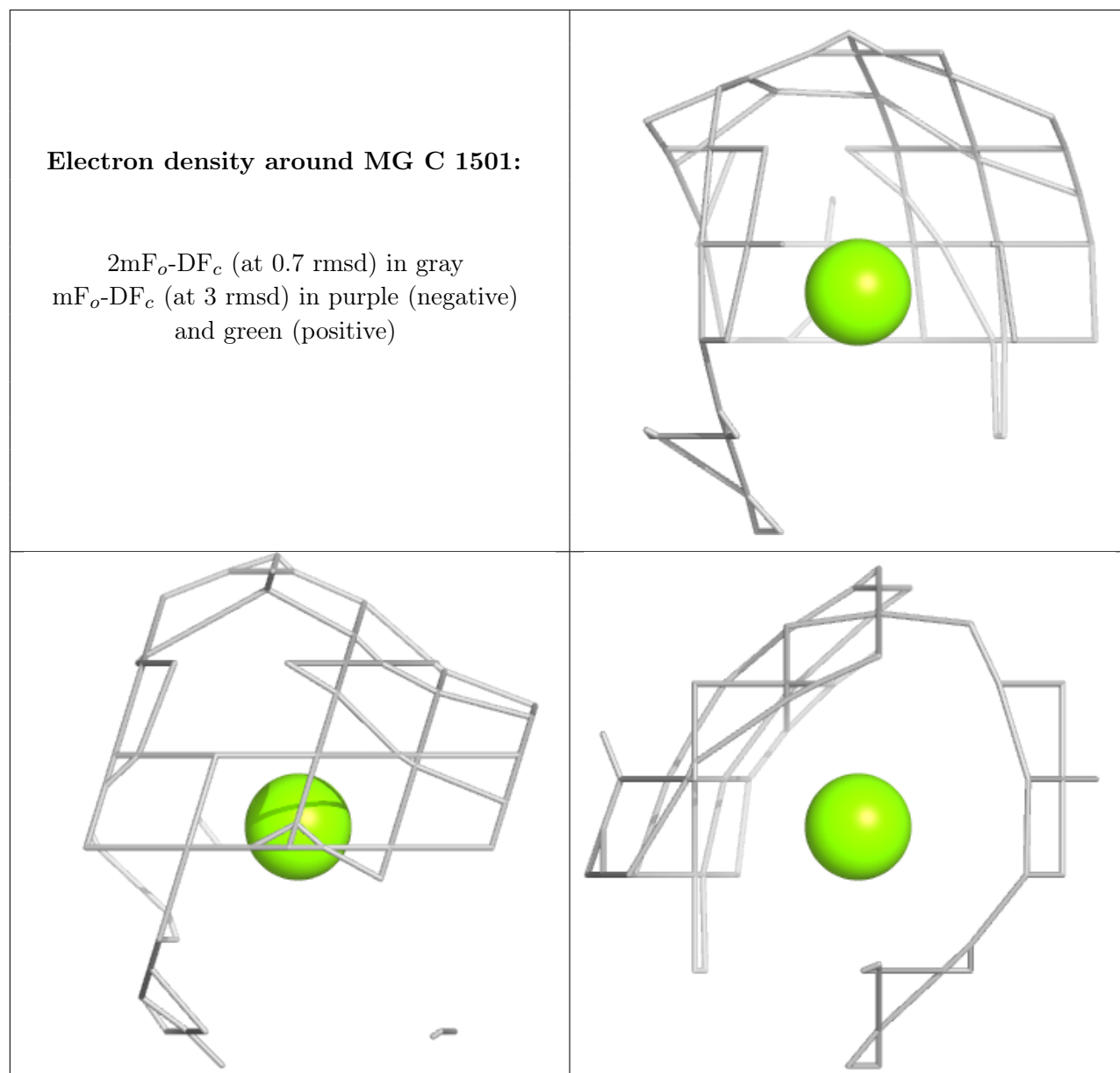
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG D 1501:

$2mF_o-DF_c$ (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.