



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2022 – 06:04 PM JST

PDB ID : 7W79  
Title : Heme exporter HrtBA in complex with Mn-AMPPNP  
Authors : Hisano, T.; Nakamura, H.; Rahman, M.M.; Tosha, T.; Shirouzu, M.; Shiro, Y.  
Deposited on : 2021-12-04  
Resolution : 3.10 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](mailto: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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

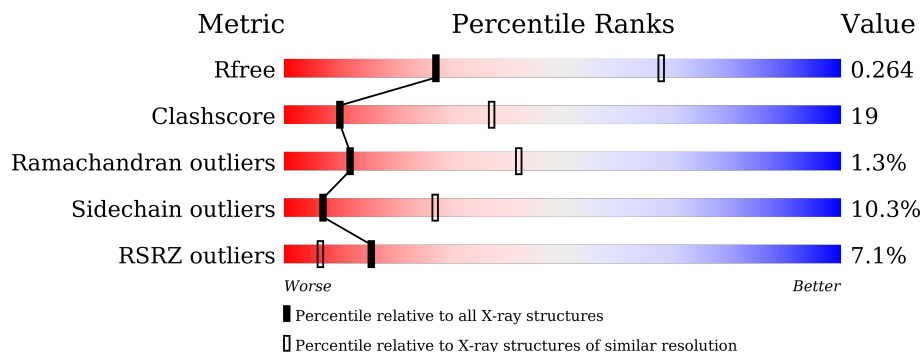
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

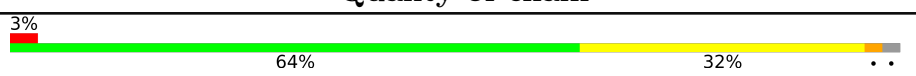

The reported resolution of this entry is 3.10 Å.

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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	221	 3% 64% 32% ..
2	B	344	 10% 63% 31% 6% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MN	B	401	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4164 atoms, of which 12 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.

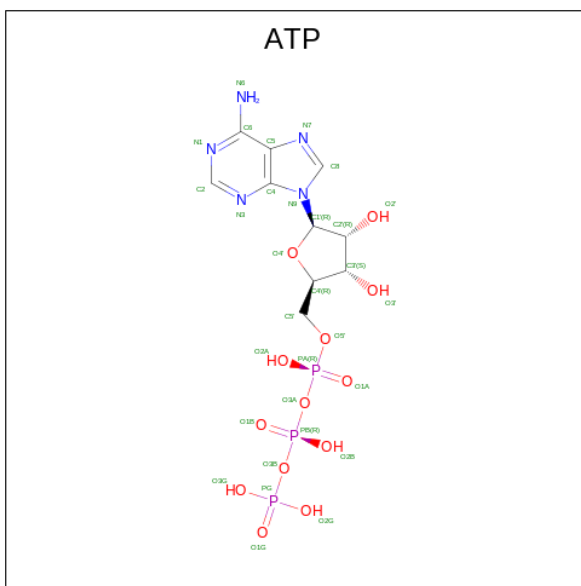
- Molecule 1 is a protein called Putative ABC transport system, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1614	1008	293	310	3	0	0	0

- Molecule 2 is a protein called Putative ABC transport system integral membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	344	2502	1608	422	467	5	0	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
3	A	1	43	10	12	5	13	3	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as

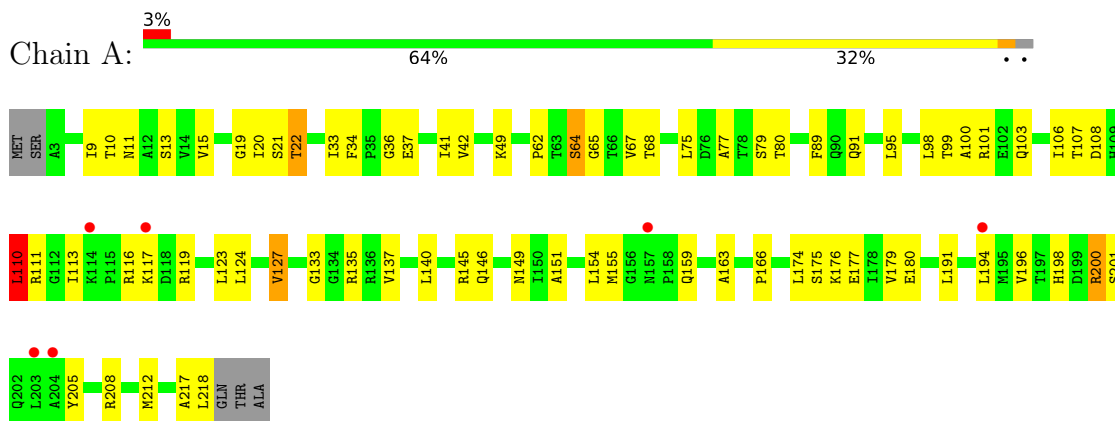
"Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	Mn 4	0	0
4	B	1	Total 1	Mn 1	0	0

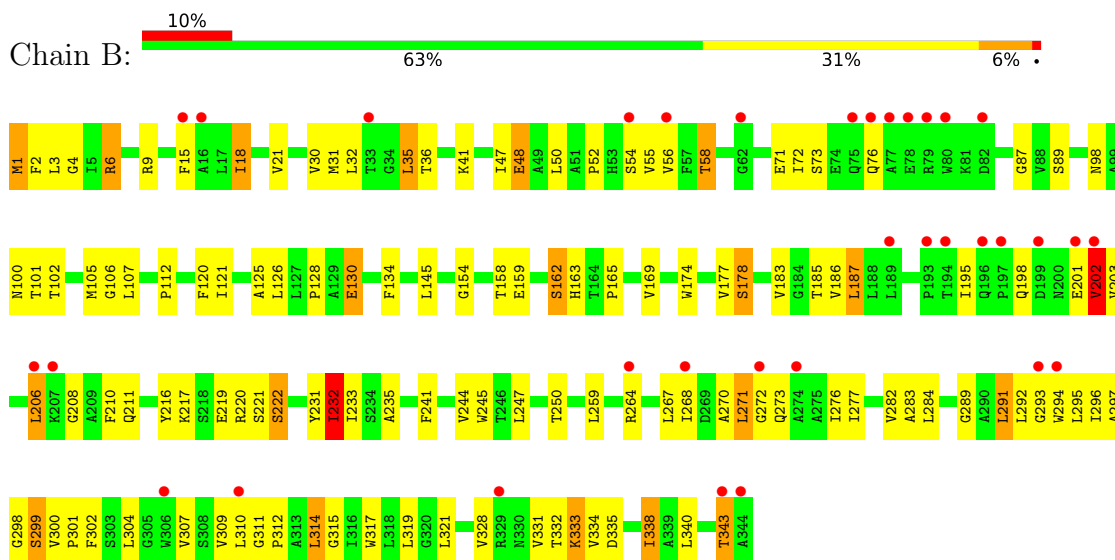
### 3 Residue-property plots i

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: Putative ABC transport system, ATP-binding protein



- Molecule 2: Putative ABC transport system integral membrane protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.37Å 169.37Å 95.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 3.10 48.54 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.54-3.10) 93.3 (48.54-2.99)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.220 , 0.261 0.221 , 0.264	Depositor DCC
$R_{free}$ test set	2000 reflections (7.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 70.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	4164	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: ATP, MN

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	0.45	0/1633	0.66	1/2211 (0.0%)
2	B	0.42	0/2548	0.62	0/3487
All	All	0.43	0/4181	0.64	1/5698 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	LEU	CA-CB-CG	7.90	133.48	115.30

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	1614	0	1659	54	0
2	B	2502	0	2559	108	0
3	A	31	12	12	0	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
All	All	4152	12	4230	159	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 19.

All (159) 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:41:ILE:HD11	1:A:194:LEU:HD22	1.42	1.02
1:A:107:THR:HA	1:A:110:LEU:HD13	1.57	0.88
2:B:56:VAL:CG1	2:B:187:LEU:HB2	2.04	0.87
1:A:107:THR:HA	1:A:110:LEU:CD1	2.05	0.87
2:B:340:LEU:O	2:B:343:THR:HG22	1.79	0.81
1:A:108:ASP:OD1	1:A:116:ARG:NH1	2.14	0.81
1:A:101:ARG:HH21	1:A:117:LYS:HB3	1.53	0.74
1:A:75:LEU:HD22	1:A:79:SER:HB2	1.68	0.73
2:B:247:LEU:O	2:B:250:THR:HG23	1.89	0.73
2:B:272:GLY:O	2:B:276:ILE:HD12	1.89	0.71
2:B:87:GLY:O	2:B:105:MET:HA	1.91	0.71
2:B:41:LYS:HE2	2:B:48:GLU:OE2	1.92	0.70
2:B:198:GLN:N	2:B:198:GLN:OE1	2.25	0.69
1:A:15:VAL:HG12	1:A:22:THR:HG22	1.74	0.68
2:B:296:ILE:HG12	2:B:296:ILE:O	1.95	0.67
2:B:47:ILE:HA	2:B:50:LEU:HD12	1.76	0.67
2:B:333:LYS:HD2	2:B:334:VAL:CG2	2.25	0.66
2:B:1:MET:SD	2:B:272:GLY:HA3	2.35	0.66
2:B:100:ASN:HB2	2:B:134:PHE:HE2	1.60	0.66
2:B:31:MET:HE3	2:B:289:GLY:HA2	1.78	0.66
2:B:334:VAL:CG1	2:B:338:ILE:HD12	2.26	0.65
2:B:4:GLY:O	2:B:273:GLN:NE2	2.27	0.65
2:B:298:GLY:H	2:B:300:VAL:H	1.45	0.65
2:B:309:VAL:HG23	2:B:310:LEU:H	1.62	0.65
2:B:56:VAL:HG12	2:B:187:LEU:HB2	1.77	0.65
1:A:123:LEU:O	1:A:127:VAL:HG22	1.97	0.65
1:A:15:VAL:HG12	1:A:22:THR:CG2	2.27	0.64
1:A:20:ILE:HG22	1:A:21:SER:N	2.12	0.64
1:A:99:THR:O	1:A:103:GLN:HG2	1.98	0.64
2:B:128:PRO:HG2	2:B:165:PRO:HB2	1.80	0.63
1:A:11:ASN:O	1:A:65:GLY:HA3	1.98	0.63
2:B:206:LEU:HD12	2:B:206:LEU:O	1.97	0.63
2:B:292:LEU:HD23	2:B:292:LEU:O	1.99	0.62
2:B:312:PRO:O	2:B:315:GLY:N	2.31	0.62
2:B:219:GLU:O	2:B:222:SER:N	2.33	0.62
2:B:145:LEU:HD23	2:B:177:VAL:HG21	1.83	0.61
1:A:176:LYS:HE2	1:A:180:GLU:OE2	2.01	0.61
1:A:89:PHE:HE2	2:B:259:LEU:HD21	1.66	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:ALA:HA	2:B:169:VAL:HG12	1.83	0.60
1:A:180:GLU:HG3	1:A:205:TYR:CE2	2.36	0.60
1:A:33:ILE:CD1	1:A:194:LEU:HG	2.31	0.60
1:A:175:SER:O	1:A:179:VAL:HG12	2.01	0.59
2:B:56:VAL:HG13	2:B:187:LEU:HB2	1.85	0.59
2:B:18:ILE:HG23	2:B:277:ILE:HG21	1.84	0.58
2:B:15:PHE:CE2	2:B:245:TRP:HZ2	2.20	0.58
2:B:293:GLY:O	2:B:296:ILE:HG22	2.04	0.58
2:B:130:GLU:OE2	2:B:158:THR:HG21	2.04	0.58
2:B:174:TRP:O	2:B:178:SER:OG	2.22	0.57
2:B:333:LYS:HD2	2:B:334:VAL:HG22	1.85	0.57
1:A:127:VAL:HG21	1:A:151:ALA:HB2	1.86	0.57
2:B:267:LEU:HG	2:B:271:LEU:HD22	1.86	0.57
1:A:49:LYS:HD2	1:A:196:VAL:HG13	1.85	0.56
2:B:298:GLY:N	2:B:300:VAL:H	2.04	0.56
1:A:108:ASP:OD2	1:A:116:ARG:HD3	2.04	0.56
2:B:264:ARG:O	2:B:268:ILE:HG12	2.05	0.56
2:B:15:PHE:HD2	2:B:277:ILE:HG13	1.70	0.55
1:A:42:VAL:HG11	1:A:200:ARG:HE	1.72	0.55
2:B:54:SER:HB3	2:B:203:VAL:CG1	2.37	0.54
1:A:163:ALA:HB1	1:A:166:PRO:HG3	1.89	0.54
2:B:2:PHE:O	2:B:6:ARG:HG2	2.08	0.54
2:B:18:ILE:CG2	2:B:277:ILE:HG21	2.38	0.54
1:A:119:ARG:NH1	1:A:155:MET:O	2.42	0.53
2:B:162:SER:O	2:B:163:HIS:HB2	2.09	0.53
2:B:302:PHE:CE1	2:B:304:LEU:HB2	2.44	0.53
2:B:89:SER:HG	2:B:174:TRP:HE1	1.54	0.53
1:A:101:ARG:NH2	1:A:117:LYS:HB3	2.22	0.52
2:B:250:THR:HG22	2:B:331:VAL:HG21	1.92	0.52
1:A:217:ALA:C	1:A:218:LEU:HD23	2.30	0.52
2:B:298:GLY:CA	2:B:300:VAL:H	2.23	0.52
2:B:106:GLY:HA2	2:B:169:VAL:O	2.09	0.51
2:B:250:THR:HG22	2:B:331:VAL:CG2	2.40	0.51
1:A:100:ALA:HB3	1:A:133:GLY:HA2	1.93	0.51
2:B:208:GLY:O	2:B:211:GLN:HB2	2.11	0.51
2:B:335:ASP:O	2:B:338:ILE:HG13	2.11	0.51
2:B:15:PHE:O	2:B:18:ILE:HG22	2.12	0.50
2:B:310:LEU:HD23	2:B:310:LEU:N	2.26	0.50
2:B:235:ALA:HA	2:B:319:LEU:HD13	1.92	0.50
1:A:107:THR:HB	1:A:111:ARG:HH12	1.77	0.50
2:B:52:PRO:HD2	2:B:206:LEU:HD22	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:HG12	1:A:67:VAL:HG22	1.94	0.49
2:B:126:LEU:HA	2:B:154:GLY:O	2.11	0.49
1:A:42:VAL:HG11	1:A:200:ARG:NE	2.27	0.49
2:B:107:LEU:HB2	2:B:121:ILE:HG13	1.92	0.49
2:B:231:TYR:CD1	2:B:231:TYR:N	2.80	0.49
2:B:270:ALA:CB	2:B:328:VAL:HG21	2.42	0.49
1:A:75:LEU:HD22	1:A:79:SER:CB	2.42	0.49
2:B:334:VAL:HG12	2:B:338:ILE:HD12	1.94	0.48
2:B:30:VAL:HG13	2:B:309:VAL:HG12	1.95	0.48
1:A:33:ILE:HD11	1:A:194:LEU:HD11	1.96	0.47
2:B:158:THR:HG23	2:B:165:PRO:HB3	1.94	0.47
2:B:206:LEU:HD12	2:B:210:PHE:CE1	2.50	0.47
1:A:180:GLU:HG3	1:A:205:TYR:HE2	1.79	0.47
2:B:201:GLU:C	2:B:202:VAL:HG12	2.35	0.47
2:B:307:VAL:HG12	2:B:307:VAL:O	2.15	0.47
2:B:317:TRP:O	2:B:321:LEU:HG	2.14	0.47
2:B:30:VAL:HG13	2:B:304:LEU:HD21	1.96	0.47
2:B:18:ILE:HG23	2:B:277:ILE:CG2	2.45	0.46
2:B:72:ILE:HD13	2:B:185:THR:C	2.36	0.46
2:B:35:LEU:HD23	2:B:302:PHE:HD2	1.80	0.46
2:B:159:GLU:HA	2:B:159:GLU:OE2	2.16	0.46
2:B:54:SER:HB3	2:B:203:VAL:HG13	1.96	0.46
2:B:299:SER:O	2:B:300:VAL:HG23	2.16	0.46
1:A:49:LYS:HD2	1:A:196:VAL:CG1	2.46	0.45
2:B:58:THR:O	2:B:58:THR:HG22	2.15	0.45
2:B:31:MET:CE	2:B:289:GLY:HA2	2.44	0.45
2:B:72:ILE:HD13	2:B:186:VAL:N	2.31	0.45
2:B:231:TYR:N	2:B:231:TYR:HD1	2.14	0.45
2:B:309:VAL:HG23	2:B:310:LEU:N	2.29	0.45
2:B:309:VAL:O	2:B:312:PRO:HD2	2.17	0.45
1:A:135:ARG:HB2	1:A:140:LEU:HD21	1.98	0.45
2:B:206:LEU:CD1	2:B:210:PHE:CE1	2.99	0.45
2:B:72:ILE:HG23	2:B:76:GLN:HB3	1.99	0.45
2:B:72:ILE:O	2:B:183:VAL:HG22	2.18	0.44
2:B:235:ALA:CB	2:B:319:LEU:HD13	2.48	0.44
2:B:334:VAL:HG12	2:B:335:ASP:N	2.32	0.44
2:B:277:ILE:HD13	2:B:277:ILE:HA	1.70	0.44
2:B:21:VAL:HG21	2:B:241:PHE:CZ	2.52	0.44
1:A:217:ALA:O	1:A:218:LEU:HD23	2.18	0.43
1:A:20:ILE:CG2	1:A:21:SER:N	2.81	0.43
2:B:235:ALA:CB	2:B:319:LEU:CD1	2.96	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:HD13	1:A:194:LEU:HG	1.99	0.43
1:A:146:GLN:O	1:A:149:ASN:HB3	2.18	0.43
1:A:34:PHE:O	1:A:37:GLU:HB2	2.19	0.42
1:A:95:LEU:HD13	2:B:3:LEU:HD22	2.00	0.42
2:B:289:GLY:O	2:B:293:GLY:N	2.47	0.42
2:B:101:THR:HG22	2:B:102:THR:N	2.34	0.42
1:A:33:ILE:CD1	1:A:194:LEU:CG	2.97	0.42
2:B:216:TYR:CZ	2:B:220:ARG:HD2	2.54	0.42
2:B:328:VAL:O	2:B:332:THR:HG23	2.19	0.42
1:A:98:LEU:HD11	1:A:106:ILE:HD12	2.02	0.42
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.74	0.42
2:B:89:SER:OG	2:B:174:TRP:NE1	2.52	0.42
2:B:217:LYS:C	2:B:219:GLU:H	2.23	0.42
1:A:89:PHE:CE2	2:B:259:LEU:HD21	2.52	0.41
2:B:35:LEU:HD23	2:B:302:PHE:CD2	2.55	0.41
2:B:112:PRO:HB3	2:B:120:PHE:CE2	2.56	0.41
2:B:31:MET:HE3	2:B:289:GLY:CA	2.45	0.41
2:B:217:LYS:O	2:B:219:GLU:N	2.53	0.41
1:A:107:THR:HB	1:A:111:ARG:NH1	2.34	0.41
2:B:32:LEU:O	2:B:36:THR:HG23	2.20	0.41
2:B:232:ILE:O	2:B:233:ILE:C	2.58	0.41
2:B:282:VAL:HG23	2:B:283:ALA:N	2.34	0.41
2:B:302:PHE:CZ	2:B:304:LEU:HD22	2.55	0.41
1:A:145:ARG:HH11	1:A:145:ARG:HD2	1.75	0.41
1:A:36:GLY:N	1:A:191:LEU:O	2.54	0.41
1:A:154:LEU:HD23	1:A:154:LEU:HA	1.83	0.41
2:B:30:VAL:CG1	2:B:309:VAL:HG12	2.51	0.41
1:A:49:LYS:HE3	1:A:198:HIS:NE2	2.36	0.41
1:A:77:ALA:O	1:A:80:THR:HB	2.21	0.41
1:A:137:VAL:HG13	1:A:145:ARG:HE	1.85	0.41
2:B:311:GLY:N	2:B:312:PRO:HD2	2.35	0.41
2:B:333:LYS:O	2:B:333:LYS:HG2	2.17	0.41
1:A:75:LEU:HA	1:A:75:LEU:HD23	1.88	0.41
2:B:333:LYS:HD2	2:B:334:VAL:HG23	1.98	0.40
1:A:62:PRO:HB2	1:A:64:SER:O	2.21	0.40
2:B:98:ASN:OD1	2:B:134:PHE:CZ	2.73	0.40
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.91	0.40
2:B:300:VAL:HG13	2:B:301:PRO:HD2	2.03	0.40
2:B:314:LEU:O	2:B:314:LEU:HG	2.21	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	A	214/221 (97%)	203 (95%)	10 (5%)	1 (0%)	29	64
2	B	342/344 (99%)	298 (87%)	38 (11%)	6 (2%)	8	34
All	All	556/565 (98%)	501 (90%)	48 (9%)	7 (1%)	12	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLY
2	B	195	ILE
2	B	297	ALA
2	B	162	SER
2	B	291	LEU
2	B	232	ILE
2	B	202	VAL

### 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	171/176 (97%)	156 (91%)	15 (9%)	10	36
2	B	257/265 (97%)	228 (89%)	29 (11%)	6	23
All	All	428/441 (97%)	384 (90%)	44 (10%)	7	27

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	13	SER
1	A	22	THR
1	A	64	SER
1	A	68	THR
1	A	91	GLN
1	A	110	LEU
1	A	113	ILE
1	A	127	VAL
1	A	159	GLN
1	A	177	GLU
1	A	200	ARG
1	A	201	SER
1	A	208	ARG
1	A	212	MET
2	B	1	MET
2	B	6	ARG
2	B	9	ARG
2	B	18	ILE
2	B	35	LEU
2	B	48	GLU
2	B	55	VAL
2	B	58	THR
2	B	71	GLU
2	B	73	SER
2	B	130	GLU
2	B	178	SER
2	B	187	LEU
2	B	202	VAL
2	B	206	LEU
2	B	221	SER
2	B	222	SER
2	B	232	ILE
2	B	244	VAL
2	B	271	LEU
2	B	284	LEU
2	B	291	LEU
2	B	294	TRP
2	B	295	LEU
2	B	299	SER
2	B	314	LEU
2	B	333	LYS
2	B	338	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	343	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	A	301	4	26,33,33	1.14	3 (11%)	31,52,52	1.34	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	301	4	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	ATP	C5-C4	2.50	1.47	1.40
3	A	301	ATP	O4'-C1'	2.48	1.44	1.41
3	A	301	ATP	C2-N3	2.05	1.35	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	ATP	N6-C6-N1	3.22	125.26	118.57
3	A	301	ATP	O3'-C3'-C4'	-2.49	103.86	111.05
3	A	301	ATP	PA-O3A-PB	-2.43	124.47	132.83
3	A	301	ATP	C2'-C3'-C4'	2.10	106.71	102.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

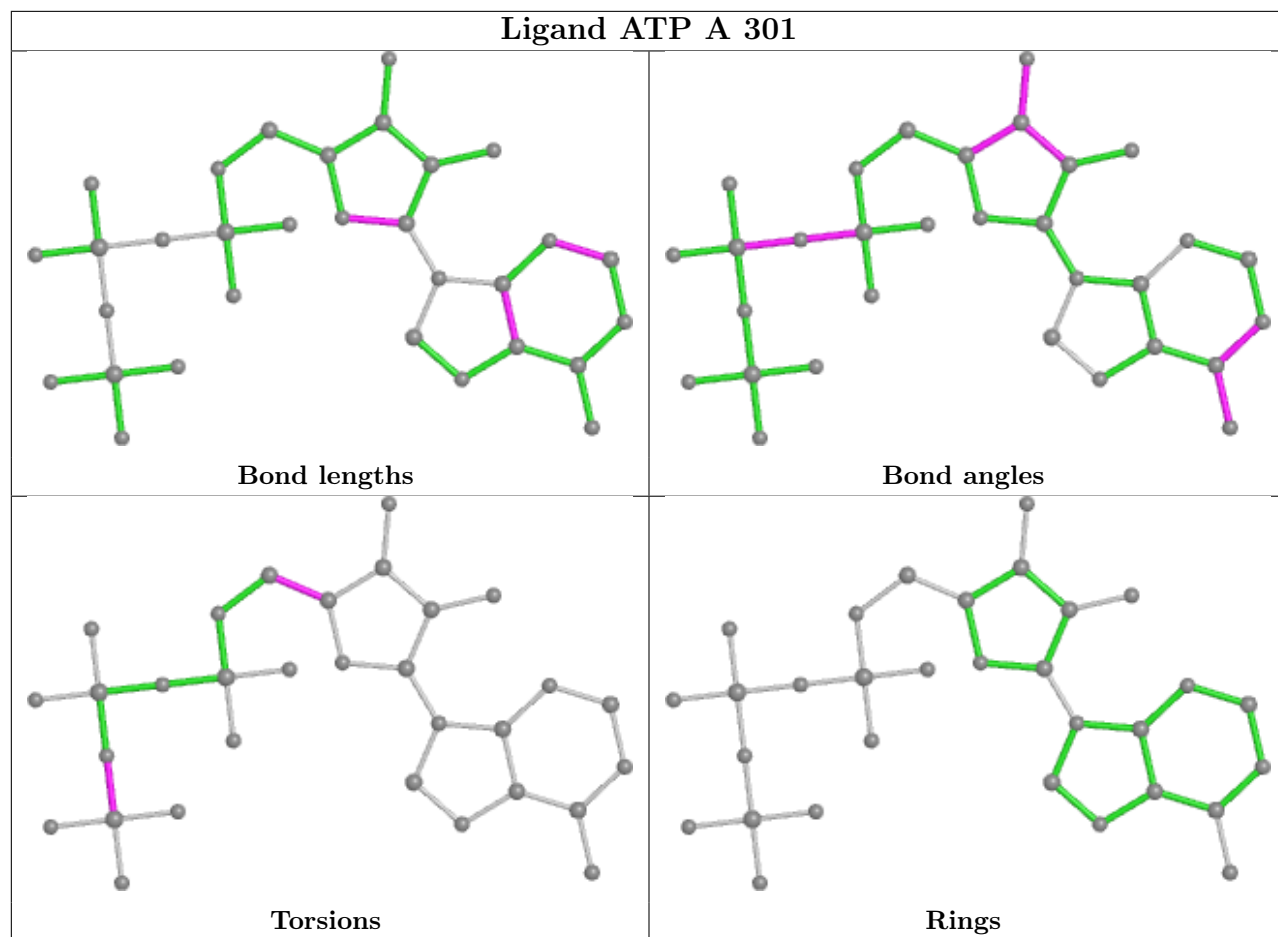
Mol	Chain	Res	Type	Atoms
3	A	301	ATP	PB-O3B-PG-O3G
3	A	301	ATP	PB-O3B-PG-O1G
3	A	301	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	216/221 (97%)	0.41	6 (2%) 53 30	64, 81, 104, 150	0
2	B	344/344 (100%)	0.63	34 (9%) 7 2	62, 91, 134, 203	0
All	All	560/565 (99%)	0.55	40 (7%) 16 6	62, 87, 128, 203	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	196	GLN	5.8
2	B	80	TRP	4.9
2	B	77	ALA	4.4
2	B	75	GLN	4.3
1	A	117	LYS	3.7
2	B	201	GLU	3.6
2	B	79	ARG	3.6
2	B	194	THR	3.5
2	B	344	ALA	3.5
2	B	268	ILE	3.3
2	B	189	LEU	3.2
2	B	78	GLU	3.2
2	B	343	THR	3.2
2	B	206	LEU	3.2
2	B	76	GLN	3.1
2	B	56	VAL	3.1
2	B	197	PRO	3.1
2	B	193	PRO	3.0
2	B	294	TRP	2.9
2	B	274	ALA	2.9
2	B	62	GLY	2.8
2	B	54	SER	2.8
2	B	306	TRP	2.7
1	A	203	LEU	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	207	LYS	2.6
2	B	82	ASP	2.6
2	B	199	ASP	2.6
1	A	157	ASN	2.4
2	B	264	ARG	2.4
1	A	114	LYS	2.3
2	B	272	GLY	2.3
2	B	15	PHE	2.3
2	B	310	LEU	2.3
1	A	204	ALA	2.2
1	A	194	LEU	2.1
2	B	33	THR	2.1
2	B	329	ARG	2.0
2	B	202	VAL	2.0
2	B	16	ALA	2.0
2	B	293	GLY	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](#)

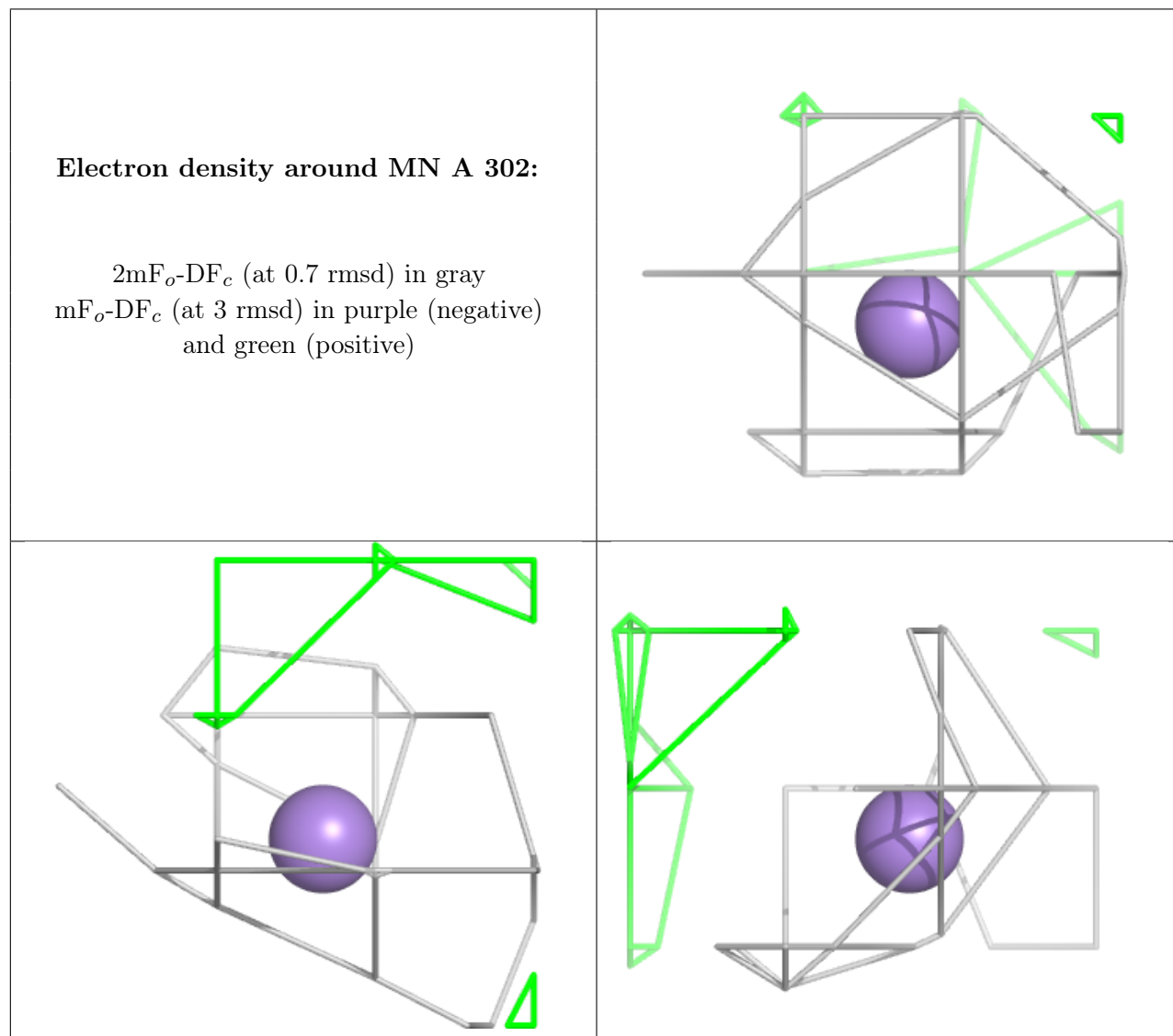
There are no monosaccharides in this entry.

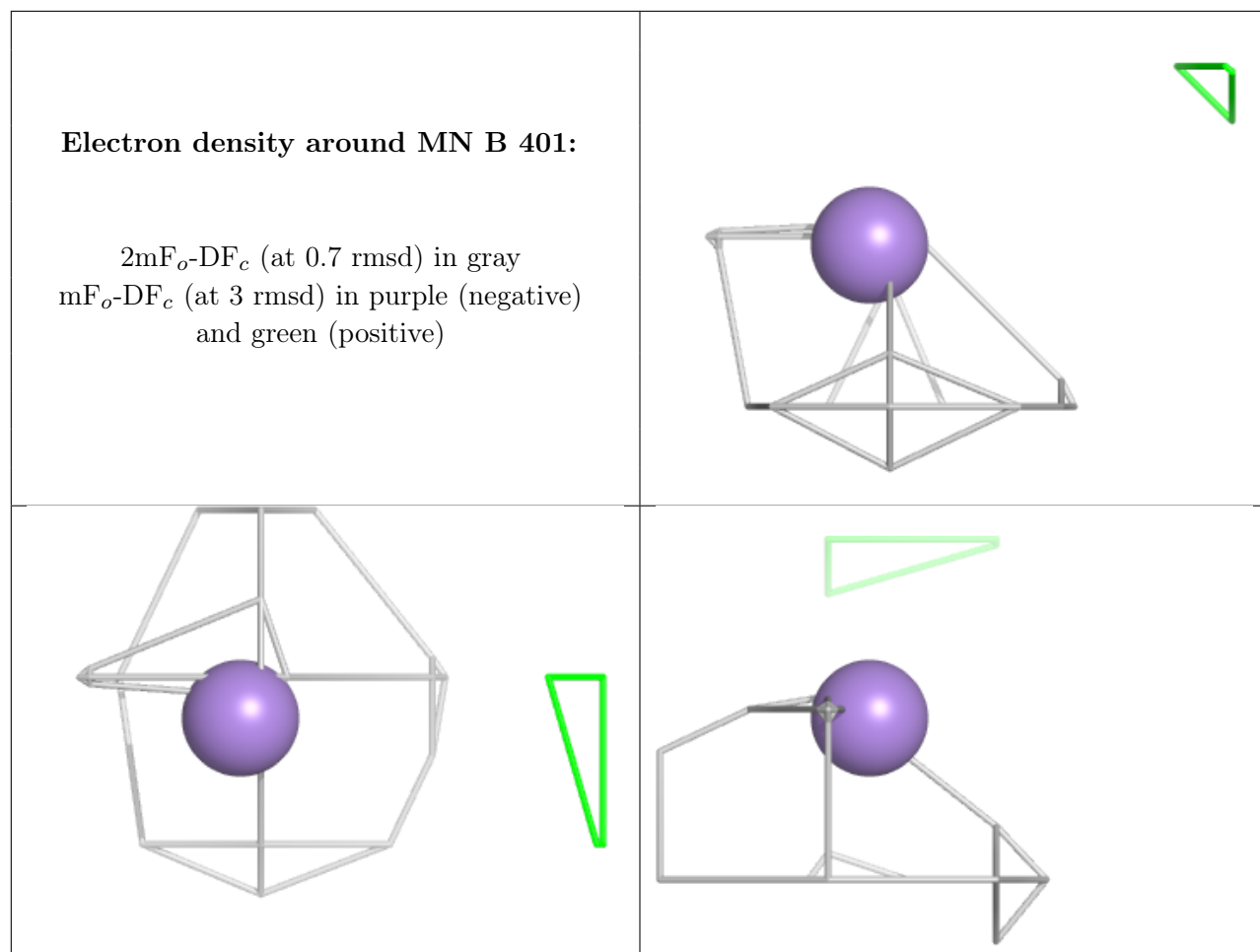
## 6.4 Ligands [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	MN	A	302	1/1	0.31	0.37	104,104,104,104	1
4	MN	B	401	1/1	0.65	0.56	90,90,90,90	1
4	MN	A	303	1/1	0.66	0.30	113,113,113,113	1
4	MN	A	304	1/1	0.92	0.08	63,63,63,63	0
3	ATP	A	301	31/31	0.94	0.21	72,72,72,72	0
4	MN	A	305	1/1	0.96	0.05	73,73,73,73	0

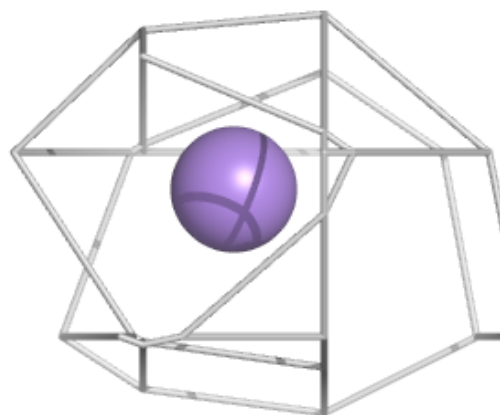
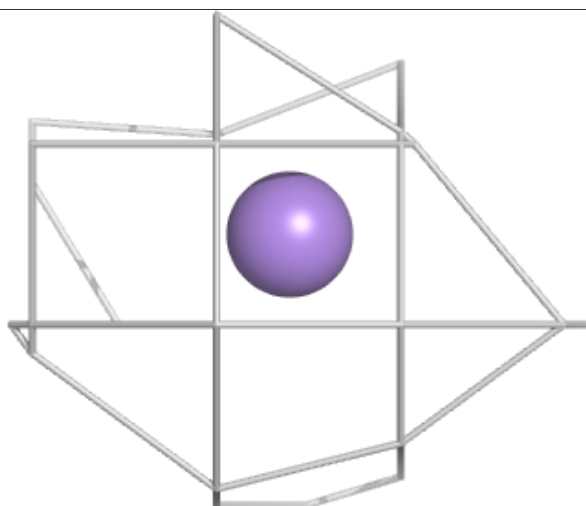
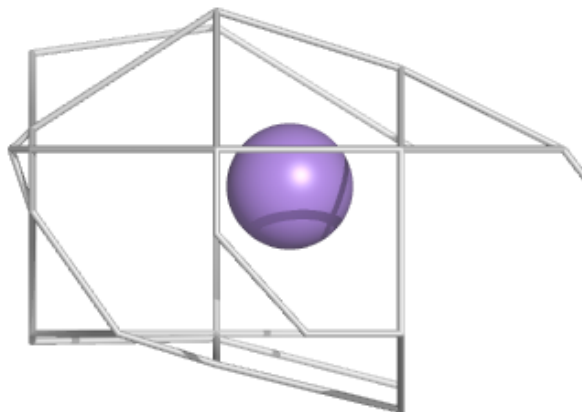
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





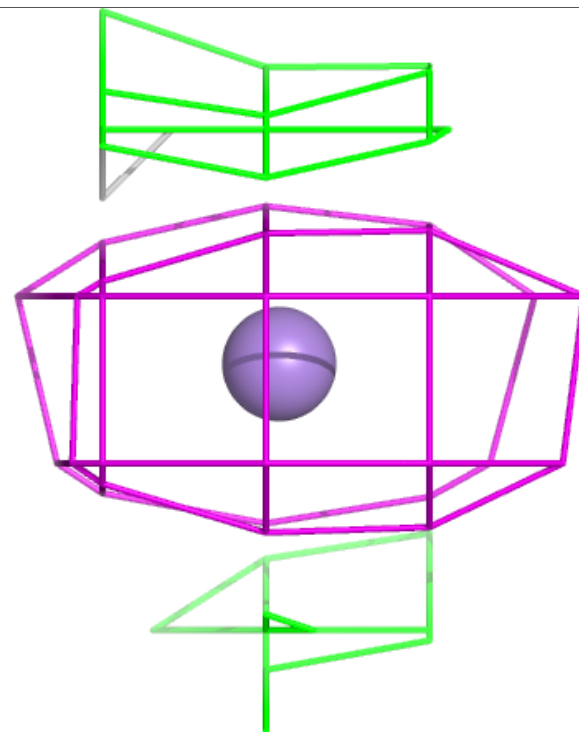
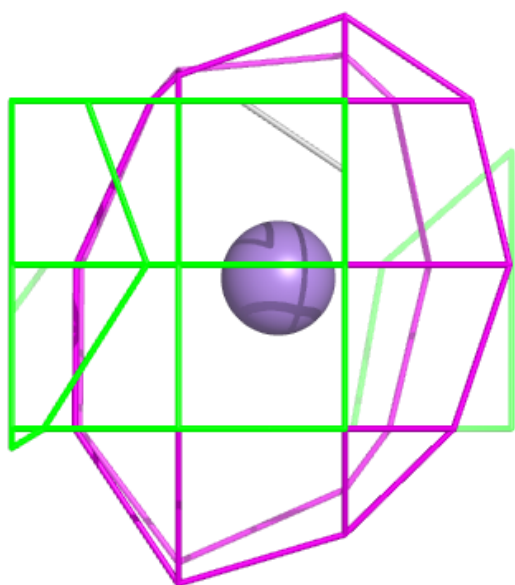
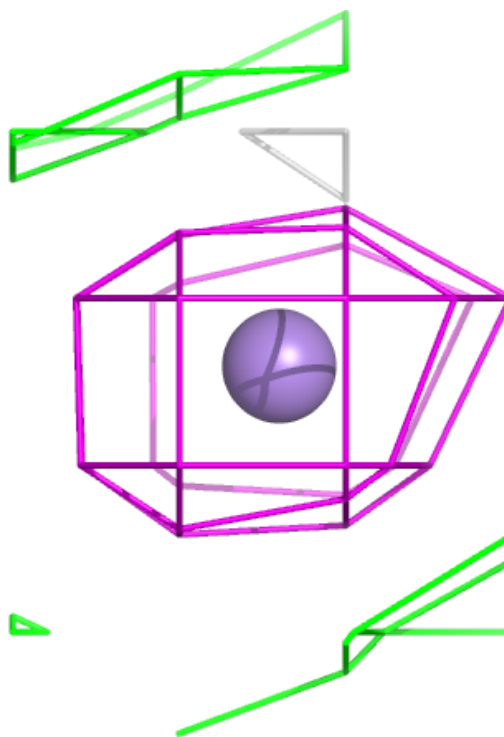
**Electron density around MN A 303:**

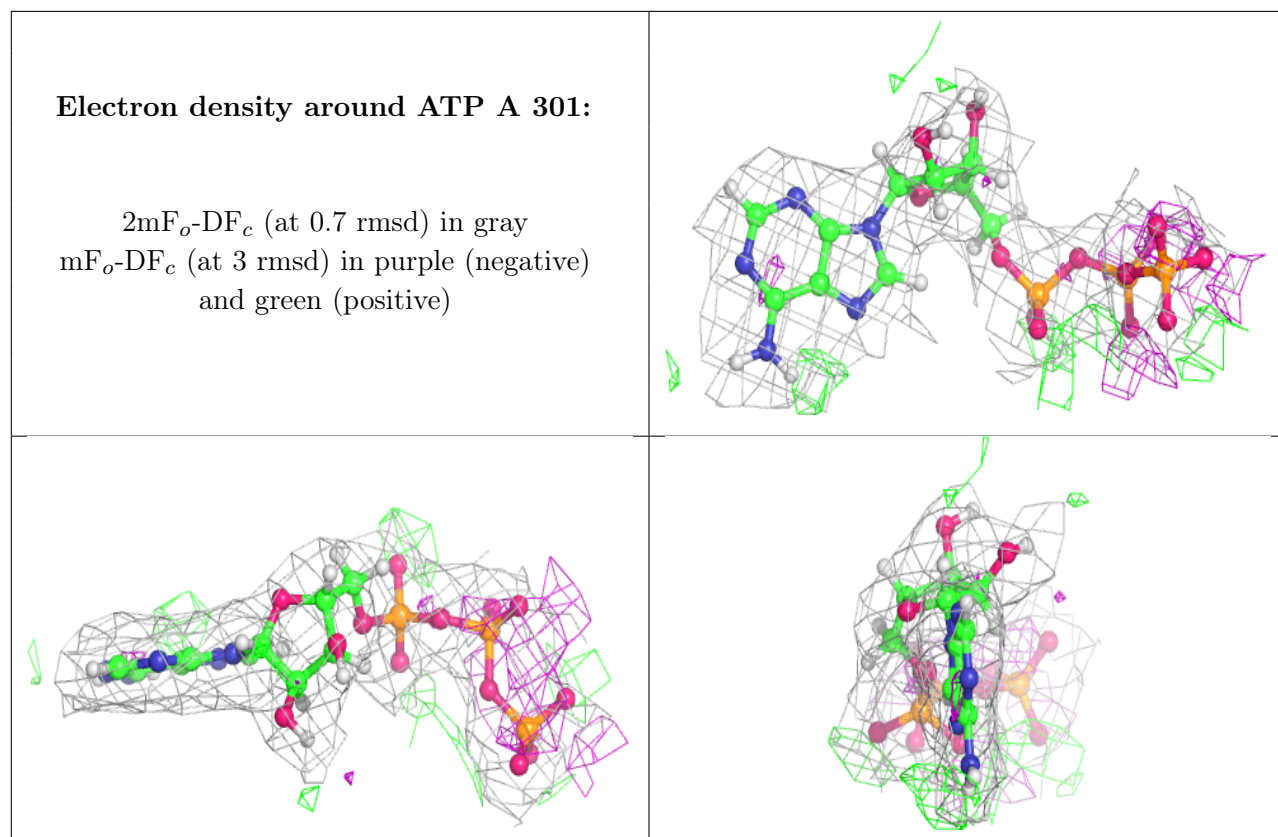
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



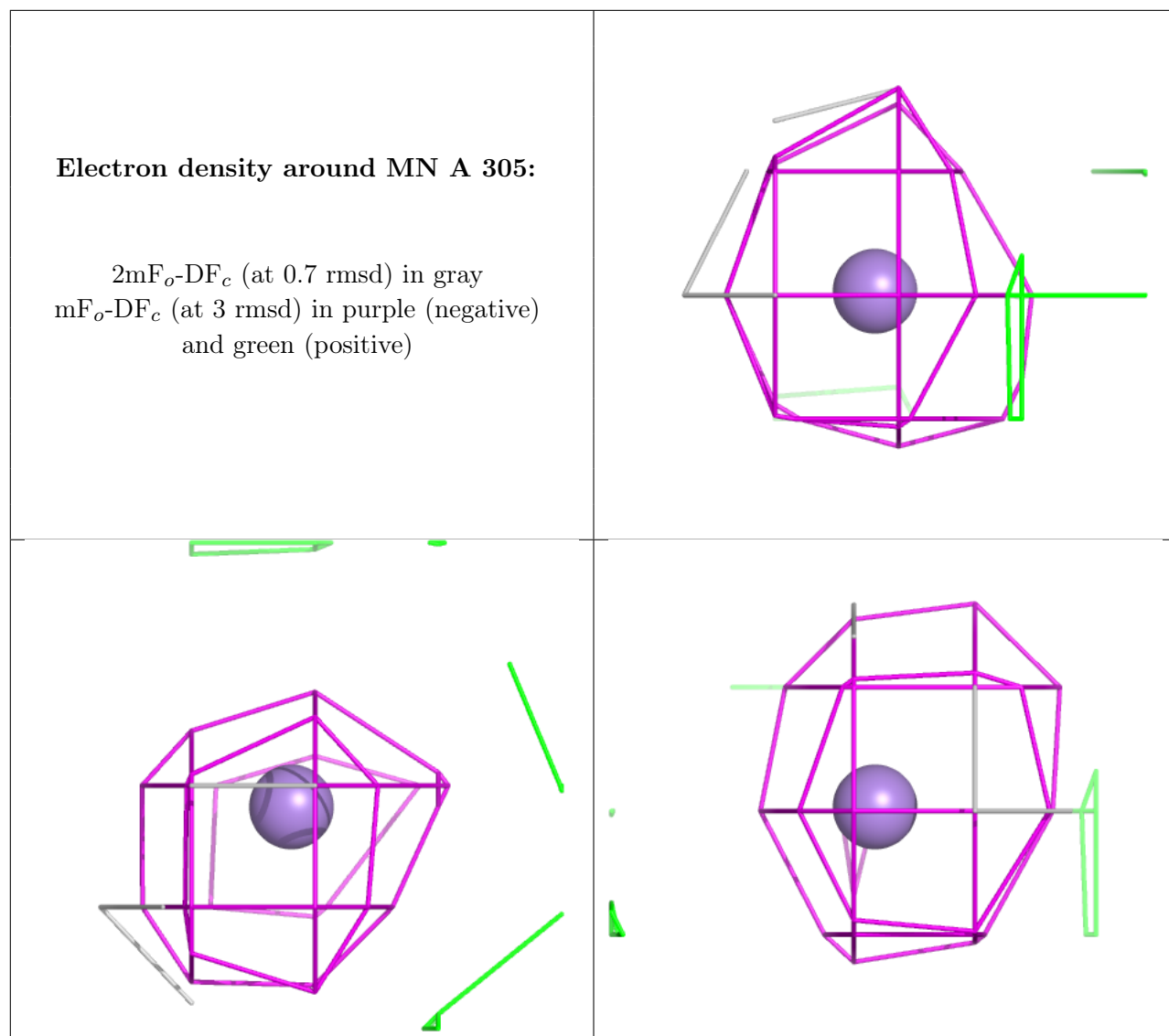
**Electron density around MN A 304:**

$2mF_o-DF_c$  (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.