



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 8, 2024 – 11:07 am BST

PDB ID : 8PMM
Title : Structure of Nall protein, allele SPIKE from japonica rice, construct 31-458
Authors : Huang, L.Y.; Rety, S.; Xi, X.G.
Deposited on : 2023-06-29
Resolution : 1.75 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 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
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

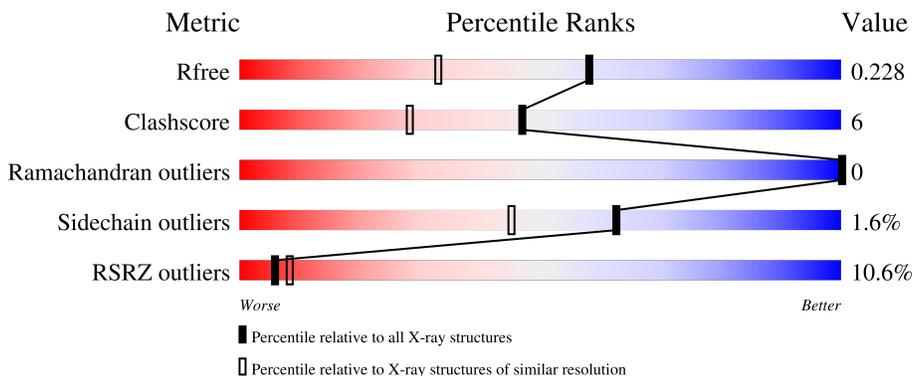
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

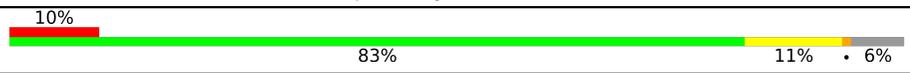
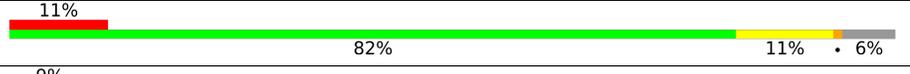
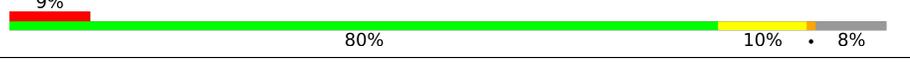
The reported resolution of this entry is 1.75 Å.

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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	433	 10% 83% 11% • 6%
1	B	433	 11% 82% 11% • 6%
1	C	433	 9% 80% 10% • 8%

2 Entry composition [i](#)

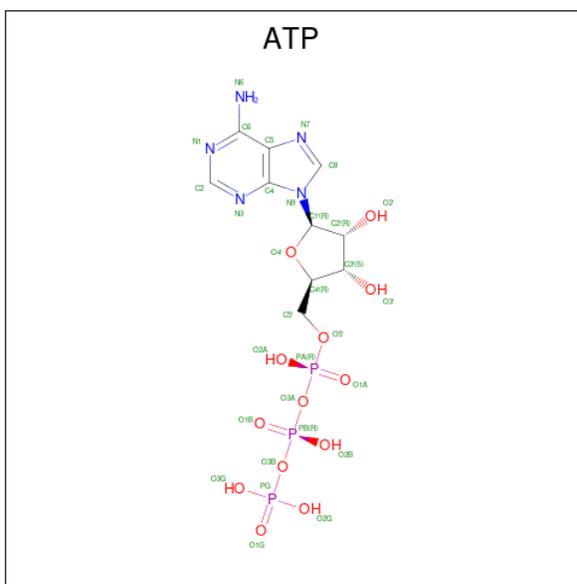
There are 5 unique types of molecules in this entry. The entry contains 10079 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protein NARROW LEAF 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	409	Total 3158	C 1998	N 553	O 594	S 13	0	0	0
1	B	408	Total 3148	C 1990	N 555	O 590	S 13	0	0	0
1	C	397	Total 3054	C 1930	N 532	O 579	S 13	0	0	0

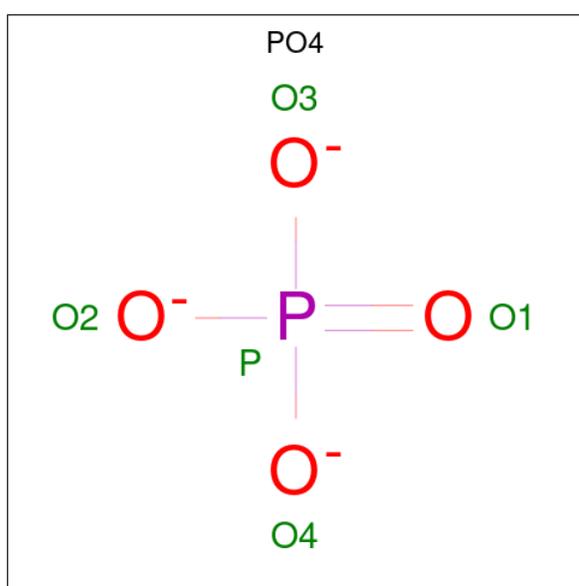
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0

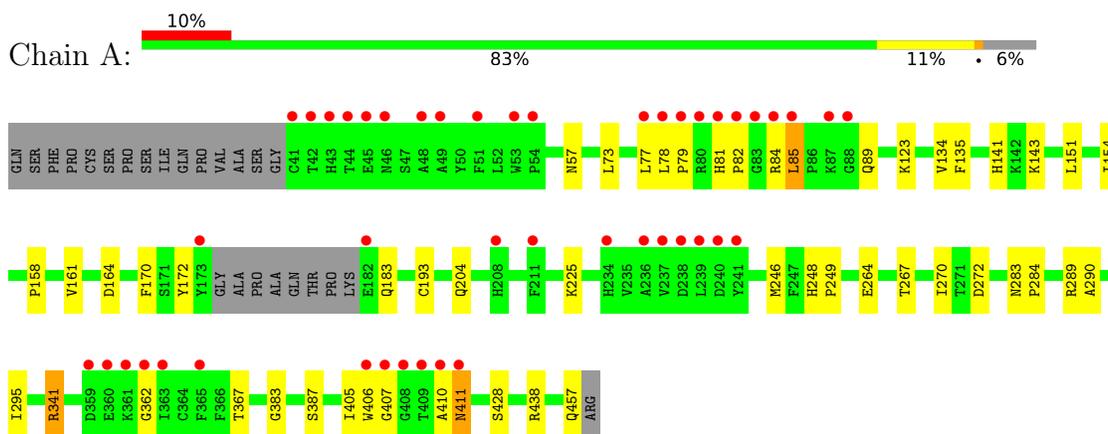
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	233	Total O 233 233	0	0
5	B	212	Total O 212 212	0	0
5	C	173	Total O 173 173	0	0

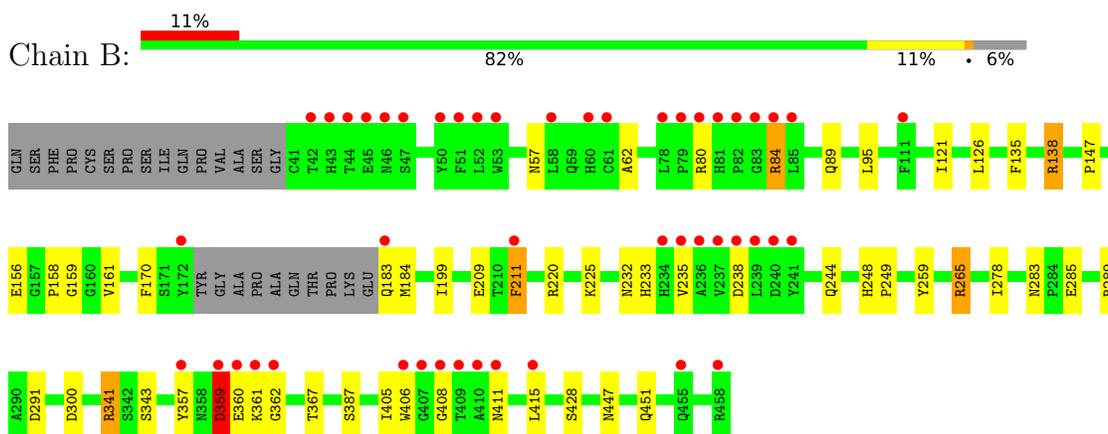
3 Residue-property plots [i](#)

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.

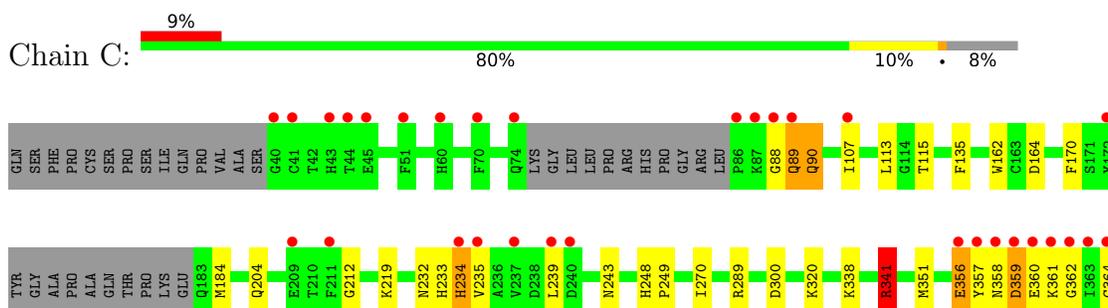
• Molecule 1: Protein NARROW LEAF 1

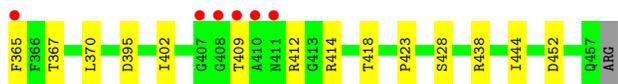


• Molecule 1: Protein NARROW LEAF 1



• Molecule 1: Protein NARROW LEAF 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	89.97Å 182.92Å 172.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.84 – 1.75 91.46 – 1.75	Depositor EDS
% Data completeness (in resolution range)	75.2 (46.84-1.75) 75.2 (91.46-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.75Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.200 , 0.231 0.198 , 0.228	Depositor DCC
R_{free} test set	5202 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtrriage
Anisotropy	0.033	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10079	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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: ATP, PO4, 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	0.31	0/3227	0.64	2/4381 (0.0%)
1	B	0.30	0/3216	0.61	1/4365 (0.0%)
1	C	0.32	0/3118	0.65	4/4231 (0.1%)
All	All	0.31	0/9561	0.63	7/12977 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	3
All	All	0	5

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	LEU	CA-CB-CG	6.17	129.50	115.30
1	B	415	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	85	LEU	CA-CB-CG	5.76	128.54	115.30
1	C	233	HIS	C-N-CA	5.69	135.93	121.70
1	C	362	GLY	N-CA-C	-5.27	99.92	113.10
1	C	89	GLN	CA-CB-CG	-5.12	102.13	113.40
1	C	359	ASP	C-N-CA	5.02	134.25	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	84	ARG	Peptide
1	B	359	ASP	Peptide
1	C	234	HIS	Peptide
1	C	341	ARG	Sidechain
1	C	356	GLU	Peptide

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	3158	0	3109	34	0
1	B	3148	0	3107	47	0
1	C	3054	0	2998	36	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
5	A	233	0	0	6	2
5	B	212	0	0	11	4
5	C	173	0	0	8	1
All	All	10079	0	9250	116	4

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 (116) 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:C:300:ASP:OD2	5:C:1101:HOH:O	1.82	0.96
1:B:220:ARG:O	5:B:1102:HOH:O	1.84	0.94
1:B:183:GLN:N	5:B:1105:HOH:O	2.06	0.86
1:C:357:TYR:HB3	1:C:365:PHE:H	1.41	0.85
1:C:243:ASN:OD1	5:C:1102:HOH:O	1.94	0.85
1:B:259:TYR:OH	5:B:1101:HOH:O	1.83	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ALA:O	5:B:1103:HOH:O	1.98	0.80
1:B:84:ARG:HD3	1:B:84:ARG:H	1.46	0.80
1:C:239:LEU:O	5:C:1103:HOH:O	1.99	0.79
1:B:367:THR:HG21	1:B:428:SER:HB2	1.66	0.76
1:C:418:THR:OG1	5:C:1105:HOH:O	2.04	0.75
1:C:395:ASP:OD2	5:C:1104:HOH:O	2.04	0.75
1:B:300:ASP:OD1	5:B:1104:HOH:O	2.04	0.74
1:A:264:GLU:OE2	5:A:1101:HOH:O	2.06	0.73
1:B:238:ASP:O	1:B:244:GLN:NE2	2.21	0.72
1:C:90:GLN:HB2	1:C:162:TRP:CE2	2.25	0.71
1:A:225:LYS:O	5:A:1102:HOH:O	2.09	0.70
1:A:367:THR:HG21	1:A:428:SER:HB2	1.73	0.69
1:B:225:LYS:HG3	5:B:1102:HOH:O	1.92	0.69
1:B:359:ASP:OD1	5:B:1106:HOH:O	2.09	0.69
1:A:457:GLN:O	5:A:1103:HOH:O	2.10	0.69
1:B:57:ASN:HD22	1:B:285:GLU:HA	1.59	0.68
1:C:204:GLN:HB2	1:C:341:ARG:HG3	1.77	0.67
1:A:283:ASN:ND2	1:A:362:GLY:O	2.29	0.66
1:B:233:HIS:N	1:B:291:ASP:OD1	2.24	0.66
1:C:452:ASP:HB2	5:C:1252:HOH:O	1.97	0.64
1:C:270:ILE:HD13	1:C:438:ARG:HG3	1.79	0.64
1:B:411:ASN:HB3	1:B:428:SER:OG	1.97	0.64
1:A:406:TRP:CZ3	1:A:411:ASN:HA	2.32	0.64
1:A:204:GLN:HB2	1:A:341:ARG:HG3	1.78	0.63
1:C:113:LEU:O	1:C:358:ASN:HB2	1.99	0.63
1:B:289:ARG:HH22	1:B:357:TYR:HD1	1.49	0.61
1:B:211:PHE:HE2	1:B:341:ARG:CZ	2.12	0.61
1:B:300:ASP:CG	5:B:1104:HOH:O	2.39	0.60
1:C:409:THR:HA	1:C:412:ARG:HG2	1.83	0.59
1:B:357:TYR:CZ	1:B:359:ASP:HB3	2.37	0.59
1:C:212:GLY:HA3	1:C:235:VAL:HG21	1.85	0.59
1:B:80:ARG:HB2	1:B:156:GLU:OE1	2.04	0.58
1:A:141:HIS:CE1	1:A:143:LYS:HG3	2.39	0.58
1:B:147:PRO:O	5:B:1107:HOH:O	2.17	0.57
1:A:81:HIS:ND1	1:A:82:PRO:HD3	2.20	0.56
1:B:406:TRP:CZ3	1:B:408:GLY:HA3	2.40	0.56
1:A:134:VAL:HG11	1:A:151:LEU:HD11	1.87	0.56
1:C:184:MET:HE2	5:C:1264:HOH:O	2.06	0.56
1:B:291:ASP:HB2	1:B:406:TRP:NE1	2.21	0.56
1:B:199:ILE:HD11	1:B:248:HIS:CD2	2.41	0.56
1:A:383:GLY:N	5:A:1104:HOH:O	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLN:OE1	1:A:341:ARG:NH1	2.37	0.54
1:C:412:ARG:HB2	1:C:414:ARG:NH2	2.23	0.54
1:B:406:TRP:HZ3	1:B:408:GLY:HA3	1.71	0.53
1:A:270:ILE:HD13	1:A:438:ARG:HG3	1.90	0.53
1:C:357:TYR:CG	1:C:358:ASN:N	2.76	0.53
1:A:81:HIS:CG	1:A:82:PRO:HD3	2.44	0.53
1:C:359:ASP:HB3	1:C:361:LYS:NZ	2.24	0.52
1:A:411:ASN:HB2	5:A:1106:HOH:O	2.08	0.52
1:B:447:ASN:O	1:B:451:GLN:HG3	2.09	0.52
1:A:77:LEU:HB3	1:A:79:PRO:HD3	1.90	0.52
1:C:107:ILE:HG23	5:C:1120:HOH:O	2.09	0.51
1:C:320:LYS:HB3	1:C:402:ILE:HG22	1.92	0.51
1:C:234:HIS:CG	1:C:234:HIS:O	2.63	0.50
1:B:184:MET:HG2	1:B:343:SER:HA	1.92	0.50
1:C:90:GLN:HB2	1:C:162:TRP:CD2	2.45	0.50
1:A:246:MET:HG3	1:A:295:ILE:HG12	1.95	0.49
1:A:81:HIS:CE1	1:A:82:PRO:HD3	2.48	0.49
1:C:115:THR:H	1:C:356:GLU:HG2	1.78	0.48
1:B:89:GLN:NE2	1:B:159:GLY:O	2.45	0.48
1:C:367:THR:HG21	1:C:428:SER:HB3	1.94	0.48
1:B:209:GLU:HG3	1:B:238:ASP:OD2	2.14	0.48
1:C:357:TYR:CD1	1:C:364:CYS:HA	2.49	0.48
1:B:80:ARG:HH12	1:B:89:GLN:HG3	1.79	0.47
1:C:135:PHE:HB3	1:C:170:PHE:HB3	1.97	0.47
1:B:158:PRO:N	5:B:1117:HOH:O	2.48	0.47
1:C:289:ARG:NE	1:C:365:PHE:HB3	2.30	0.47
1:B:357:TYR:CE1	1:B:359:ASP:HB3	2.50	0.46
1:C:351:MET:HB2	1:C:370:LEU:HD22	1.98	0.46
1:A:85:LEU:CD2	1:A:154:ILE:HG21	2.45	0.46
1:A:289:ARG:HD3	1:A:406:TRP:CZ2	2.51	0.46
1:A:387:SER:HB2	1:A:405:ILE:HD12	1.97	0.46
1:B:211:PHE:CE2	1:B:341:ARG:CZ	2.96	0.46
1:A:172:TYR:CD1	1:A:410:ALA:HB1	2.50	0.46
1:C:88:GLY:H	1:C:162:TRP:HE1	1.64	0.46
1:C:357:TYR:CB	1:C:365:PHE:H	2.22	0.45
1:A:406:TRP:CD1	1:A:407:GLY:N	2.84	0.45
1:B:84:ARG:H	1:B:84:ARG:CD	2.21	0.45
1:A:123:LYS:HD2	1:A:123:LYS:N	2.32	0.45
1:A:406:TRP:CE3	1:A:411:ASN:HA	2.53	0.44
1:C:219:LYS:HB3	1:C:444:ILE:HD11	2.00	0.44
1:B:57:ASN:ND2	1:B:285:GLU:HA	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:HIS:HA	1:A:249:PRO:HA	1.83	0.44
1:B:232:ASN:ND2	1:B:235:VAL:H	2.16	0.44
1:B:359:ASP:O	1:B:361:LYS:O	2.36	0.43
1:A:135:PHE:HB3	1:A:170:PHE:HB3	2.00	0.43
1:B:361:LYS:HD3	1:B:361:LYS:HA	1.61	0.43
1:A:57:ASN:HB2	1:A:284:PRO:O	2.19	0.43
1:A:89:GLN:O	1:A:161:VAL:HA	2.18	0.43
1:C:232:ASN:ND2	1:C:235:VAL:H	2.17	0.43
1:A:267:THR:HG23	1:A:290:ALA:O	2.19	0.43
1:B:248:HIS:HA	1:B:249:PRO:HA	1.82	0.43
1:B:135:PHE:HB3	1:B:170:PHE:HB3	2.00	0.42
1:C:357:TYR:HB3	1:C:365:PHE:N	2.22	0.42
1:C:414:ARG:HB3	1:C:423:PRO:HB2	2.00	0.42
1:A:193:CYS:SG	1:A:341:ARG:HG2	2.59	0.42
1:B:89:GLN:O	1:B:161:VAL:HA	2.18	0.42
1:B:387:SER:HB2	1:B:405:ILE:HD12	2.01	0.42
1:A:73:LEU:HD13	1:A:158:PRO:HG2	2.01	0.42
1:A:411:ASN:CB	5:A:1106:HOH:O	2.66	0.42
1:B:138:ARG:NH2	1:C:204:GLN:OE1	2.51	0.42
1:B:289:ARG:NH1	5:B:1125:HOH:O	2.53	0.41
1:A:272:ASP:N	1:A:272:ASP:OD1	2.54	0.41
1:B:265:ARG:CZ	1:B:265:ARG:HB3	2.50	0.41
1:B:95:LEU:HD11	1:B:278:ILE:HG21	2.03	0.41
1:B:121:ILE:HG12	1:B:126:LEU:HD23	2.01	0.41
1:B:283:ASN:HD21	1:B:362:GLY:C	2.24	0.41
1:C:88:GLY:HA3	1:C:162:TRP:HD1	1.85	0.41
1:C:248:HIS:HA	1:C:249:PRO:HA	1.78	0.40
1:B:283:ASN:ND2	1:B:362:GLY:O	2.50	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1187:HOH:O	5:B:1109:HOH:O[3_555]	1.97	0.23
5:B:1248:HOH:O	5:B:1284:HOH:O[3_455]	2.07	0.13
5:B:1176:HOH:O	5:C:1106:HOH:O[6_454]	2.08	0.12
5:A:1312:HOH:O	5:B:1295:HOH:O[3_555]	2.18	0.02

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	405/433 (94%)	405 (100%)	0	0	100	100
1	B	404/433 (93%)	404 (100%)	0	0	100	100
1	C	391/433 (90%)	391 (100%)	0	0	100	100
All	All	1200/1299 (92%)	1200 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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	341/360 (95%)	338 (99%)	3 (1%)	78	67
1	B	340/360 (94%)	333 (98%)	7 (2%)	53	31
1	C	330/360 (92%)	324 (98%)	6 (2%)	59	40
All	All	1011/1080 (94%)	995 (98%)	16 (2%)	62	45

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ASP
1	A	341	ARG
1	A	411	ASN
1	B	84	ARG
1	B	138	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	211	PHE
1	B	265	ARG
1	B	341	ARG
1	B	359	ASP
1	B	360	GLU
1	C	89	GLN
1	C	90	GLN
1	C	164	ASP
1	C	338	LYS
1	C	341	ARG
1	C	360	GLU

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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
2	ATP	A	1001	3	26,33,33	0.66	0	31,52,52	0.78	1 (3%)
2	ATP	B	1001	3	26,33,33	0.63	0	31,52,52	0.77	1 (3%)
2	ATP	C	1001	3	26,33,33	0.62	0	31,52,52	0.77	1 (3%)
4	PO4	A	1003	-	4,4,4	0.91	0	6,6,6	0.34	0

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
2	ATP	A	1001	3	-	2/18/38/38	0/3/3/3
2	ATP	B	1001	3	-	2/18/38/38	0/3/3/3
2	ATP	C	1001	3	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	ATP	C5-C6-N6	2.20	123.70	120.35
2	C	1001	ATP	C5-C6-N6	2.18	123.66	120.35
2	A	1001	ATP	C5-C6-N6	2.12	123.57	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

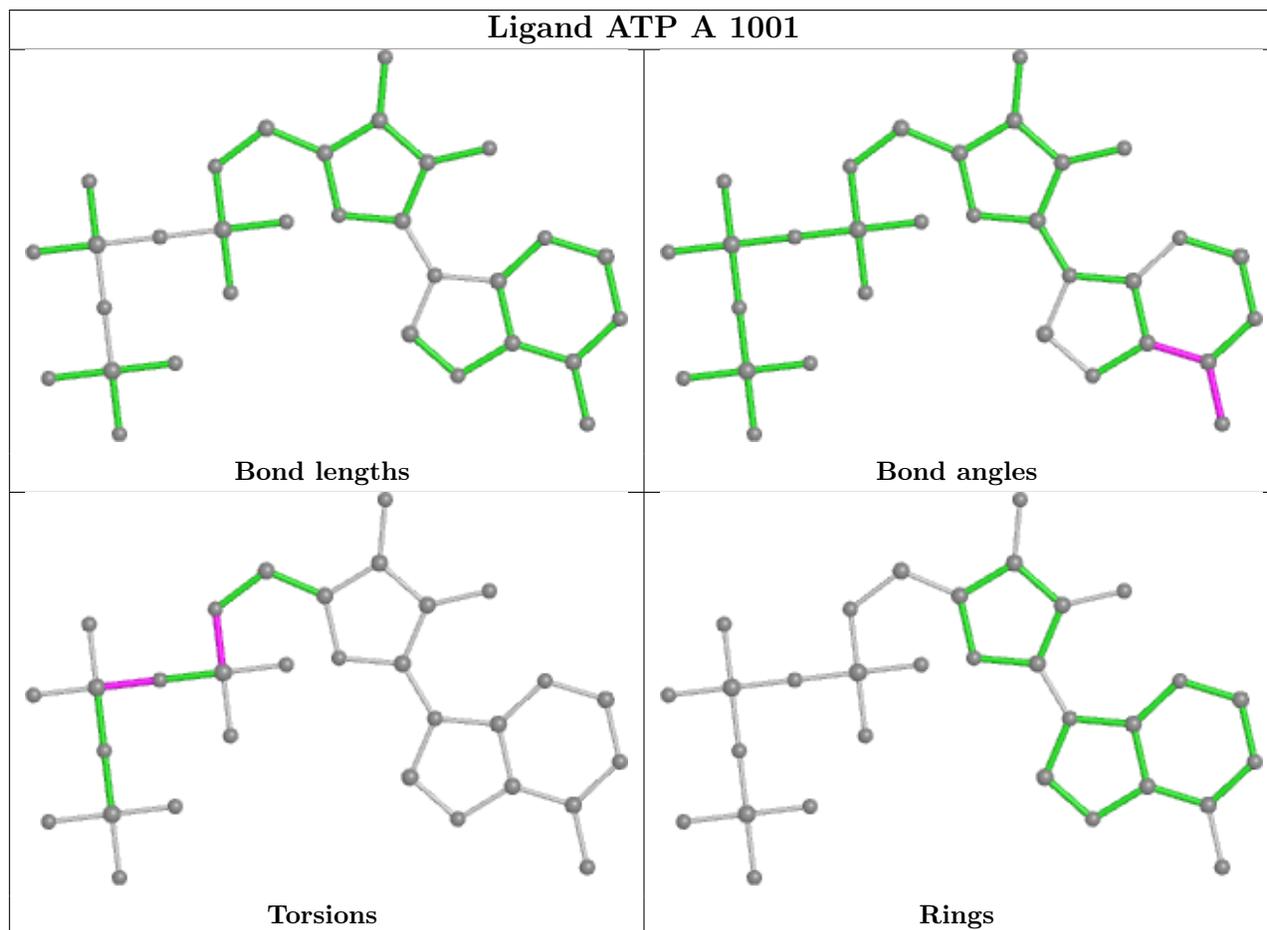
Mol	Chain	Res	Type	Atoms
2	C	1001	ATP	PA-O3A-PB-O1B
2	B	1001	ATP	PA-O3A-PB-O1B
2	A	1001	ATP	PA-O3A-PB-O1B
2	B	1001	ATP	PA-O3A-PB-O2B
2	C	1001	ATP	PA-O3A-PB-O2B
2	C	1001	ATP	PB-O3B-PG-O3G
2	A	1001	ATP	C5'-O5'-PA-O3A
2	C	1001	ATP	C5'-O5'-PA-O3A

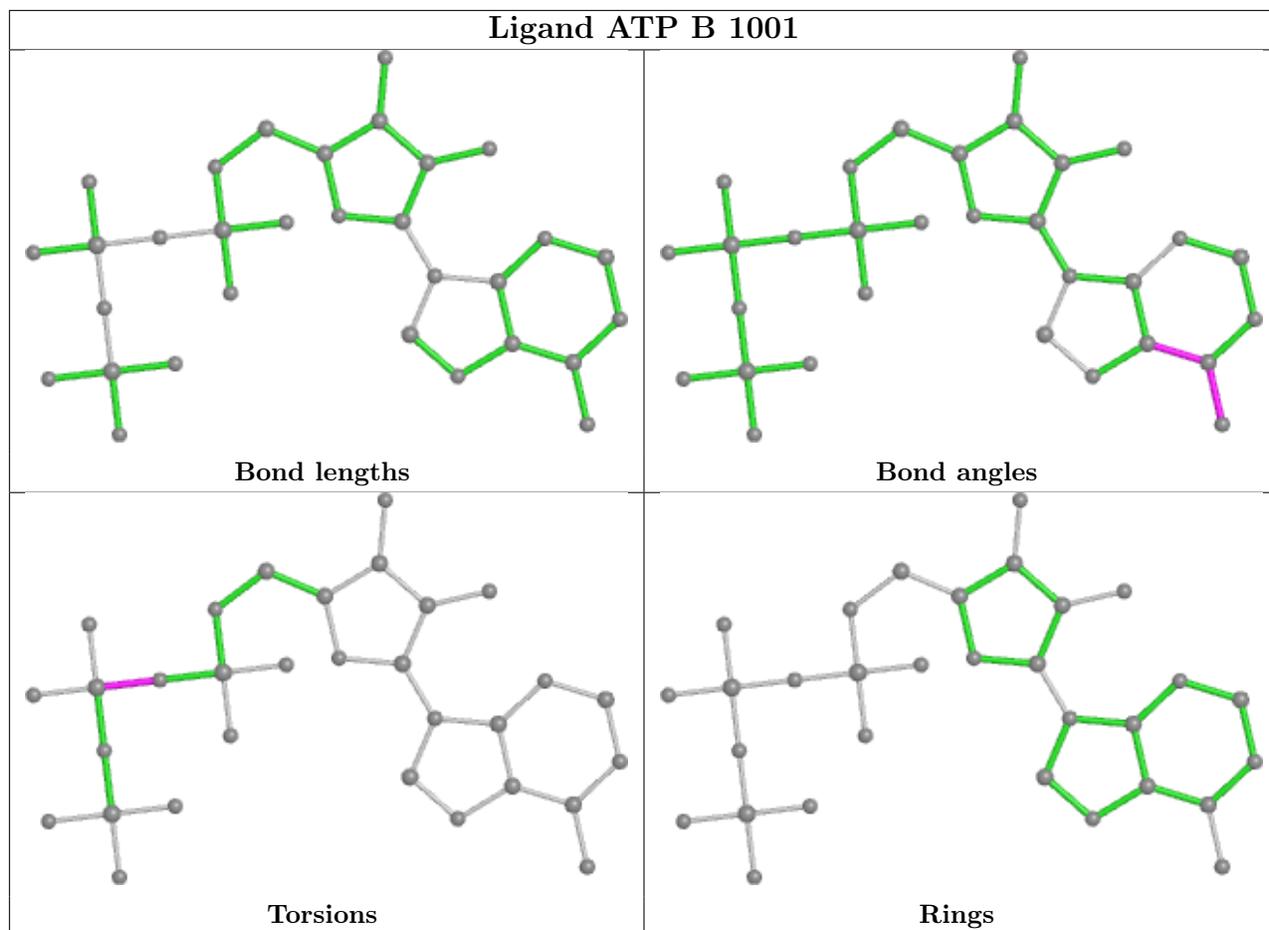
There are no ring outliers.

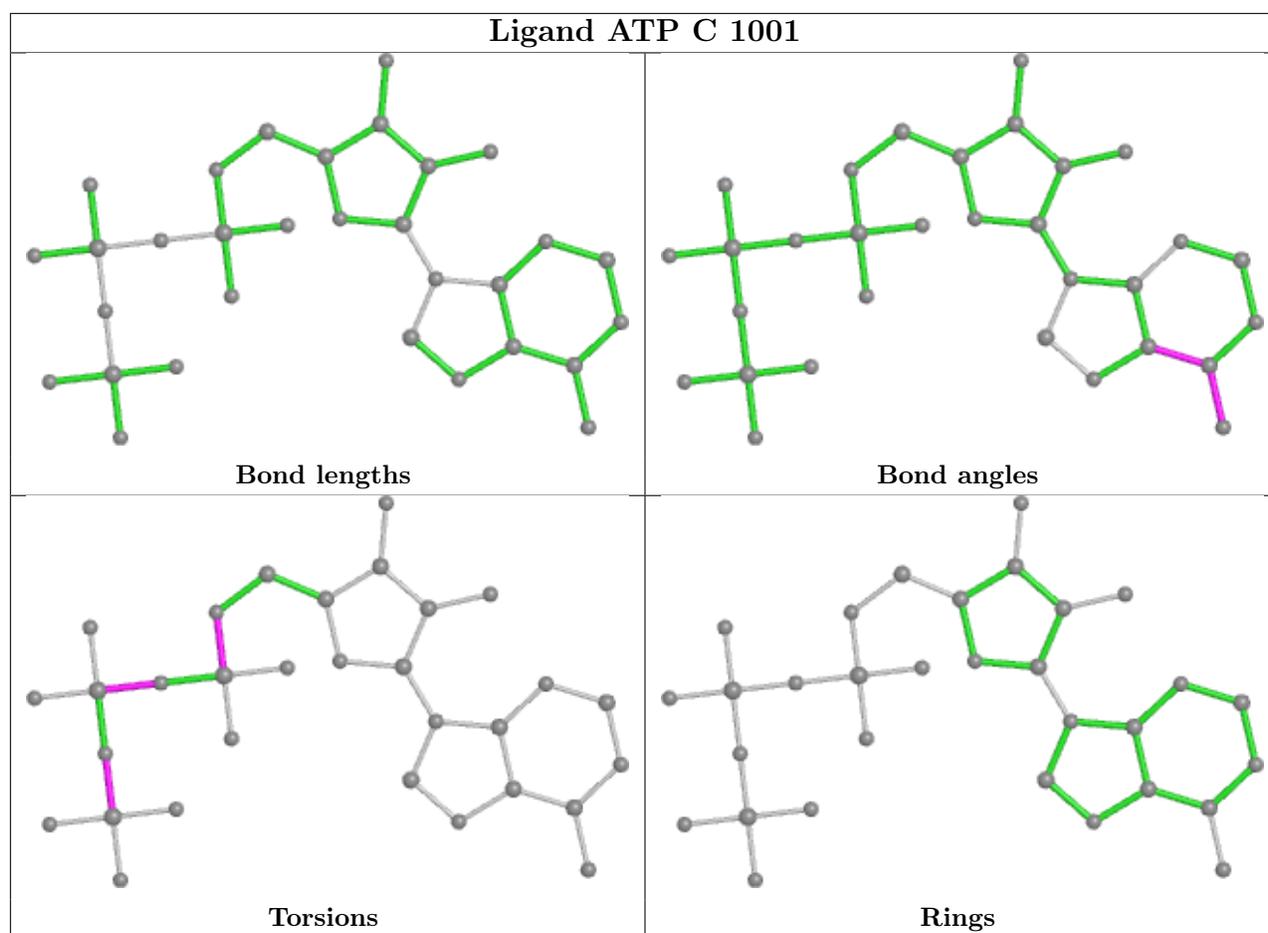
No monomer is involved in short contacts.

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, 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	409/433 (94%)	0.77	45 (11%) 5 7	19, 36, 84, 145	0
1	B	408/433 (94%)	0.64	47 (11%) 4 6	20, 38, 83, 122	0
1	C	397/433 (91%)	0.53	37 (9%) 8 11	25, 38, 75, 98	0
All	All	1214/1299 (93%)	0.65	129 (10%) 6 8	19, 38, 81, 145	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	43	HIS	16.2
1	A	82	PRO	14.9
1	A	409	THR	13.5
1	A	80	ARG	12.2
1	A	42	THR	11.5
1	A	78	LEU	10.8
1	B	44	THR	10.7
1	B	409	THR	10.6
1	A	81	HIS	10.6
1	A	44	THR	9.6
1	A	408	GLY	9.5
1	B	83	GLY	9.3
1	C	410	ALA	9.3
1	B	82	PRO	8.9
1	A	239	LEU	8.9
1	B	408	GLY	8.6
1	C	357	TYR	8.6
1	C	88	GLY	8.1
1	C	239	LEU	8.1
1	C	409	THR	8.0
1	A	362	GLY	7.9
1	B	81	HIS	7.8
1	A	407	GLY	7.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	410	ALA	6.9
1	C	358	ASN	6.8
1	B	84	ARG	6.8
1	B	362	GLY	6.6
1	C	408	GLY	6.6
1	A	79	PRO	6.5
1	C	240	ASP	6.5
1	A	85	LEU	6.5
1	B	240	ASP	6.4
1	A	77	LEU	6.0
1	B	239	LEU	5.9
1	A	45	GLU	5.8
1	C	211	PHE	5.6
1	C	411	ASN	5.5
1	C	40	GLY	5.5
1	C	363	ILE	5.4
1	A	83	GLY	5.2
1	B	361	LYS	5.2
1	A	360	GLU	5.1
1	B	237	VAL	5.0
1	B	241	TYR	5.0
1	B	407	GLY	5.0
1	C	172	TYR	4.9
1	A	411	ASN	4.8
1	C	41	CYS	4.7
1	B	111	PHE	4.6
1	C	359	ASP	4.6
1	A	41	CYS	4.5
1	B	42	THR	4.5
1	C	87	LYS	4.4
1	B	183	GLN	4.3
1	B	79	PRO	4.2
1	B	43	HIS	4.1
1	C	44	THR	4.1
1	B	211	PHE	4.1
1	B	238	ASP	4.1
1	A	51	PHE	3.9
1	B	359	ASP	3.7
1	B	53	TRP	3.6
1	C	364	CYS	3.6
1	A	410	ALA	3.5
1	C	86	PRO	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	43	HIS	3.5
1	B	411	ASN	3.4
1	B	60	HIS	3.4
1	A	236	ALA	3.4
1	C	360	GLU	3.3
1	A	84	ARG	3.3
1	A	359	ASP	3.3
1	B	80	ARG	3.3
1	B	78	LEU	3.3
1	A	365	PHE	3.2
1	A	238	ASP	3.2
1	C	237	VAL	3.2
1	C	407	GLY	3.2
1	A	237	VAL	3.1
1	B	85	LEU	3.1
1	A	241	TYR	3.0
1	A	363	ILE	3.0
1	A	48	ALA	3.0
1	B	236	ALA	2.9
1	C	234	HIS	2.9
1	B	234	HIS	2.9
1	C	361	LYS	2.8
1	A	240	ASP	2.8
1	B	45	GLU	2.8
1	A	361	LYS	2.7
1	A	406	TRP	2.7
1	B	406	TRP	2.7
1	A	49	ALA	2.6
1	B	51	PHE	2.6
1	B	47	SER	2.6
1	C	60	HIS	2.6
1	A	54	PRO	2.6
1	B	458	ARG	2.5
1	A	211	PHE	2.5
1	B	172	TYR	2.5
1	A	88	GLY	2.5
1	C	89	GLN	2.5
1	C	235	VAL	2.5
1	B	52	LEU	2.4
1	C	362	GLY	2.4
1	C	356	GLU	2.4
1	B	61	CYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	360	GLU	2.3
1	B	235	VAL	2.3
1	B	50	TYR	2.3
1	B	58	LEU	2.3
1	B	455	GLN	2.2
1	B	46	ASN	2.2
1	B	357	TYR	2.2
1	A	53	TRP	2.2
1	A	234	HIS	2.2
1	A	173	TYR	2.1
1	C	365	PHE	2.1
1	B	415	LEU	2.1
1	C	70	PHE	2.1
1	A	182	GLU	2.1
1	C	209	GLU	2.1
1	C	51	PHE	2.1
1	A	46	ASN	2.1
1	A	208	HIS	2.1
1	C	74	GLN	2.1
1	A	87	LYS	2.1
1	C	107	ILE	2.1
1	C	45	GLU	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, 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
4	PO4	A	1003	5/5	0.74	0.32	82,103,144,205	0

Continued on next page...

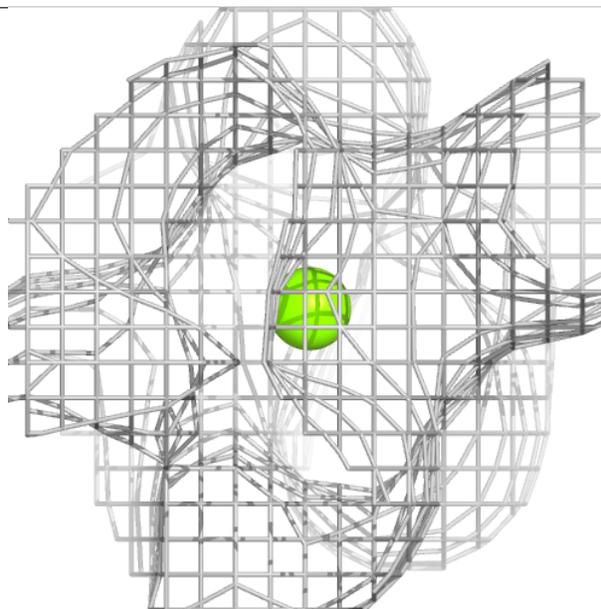
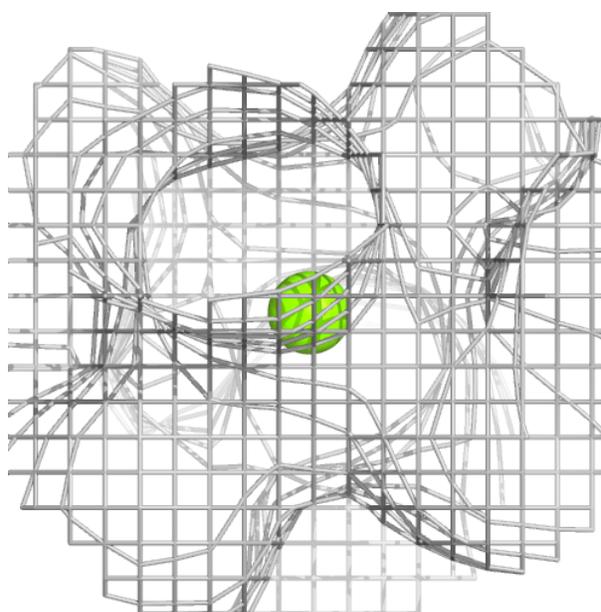
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	1002	1/1	0.97	0.11	26,26,26,26	0
2	ATP	B	1001	31/31	0.97	0.09	28,34,39,41	0
2	ATP	A	1001	31/31	0.98	0.08	24,29,33,34	0
3	MG	B	1002	1/1	0.98	0.07	29,29,29,29	0
3	MG	C	1002	1/1	0.98	0.12	25,25,25,25	0
2	ATP	C	1001	31/31	0.98	0.10	24,28,32,36	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.

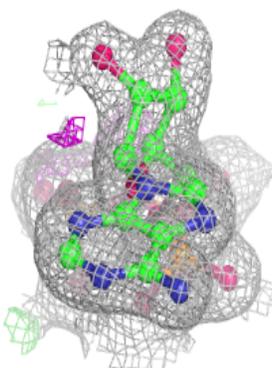
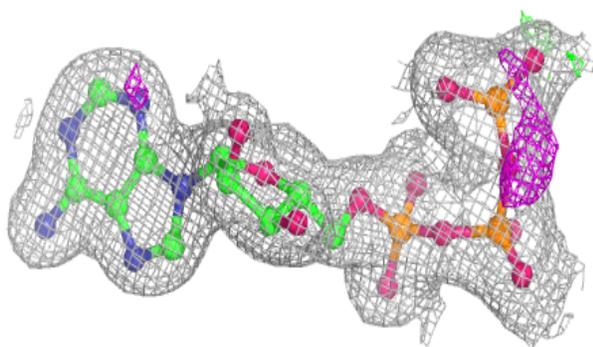
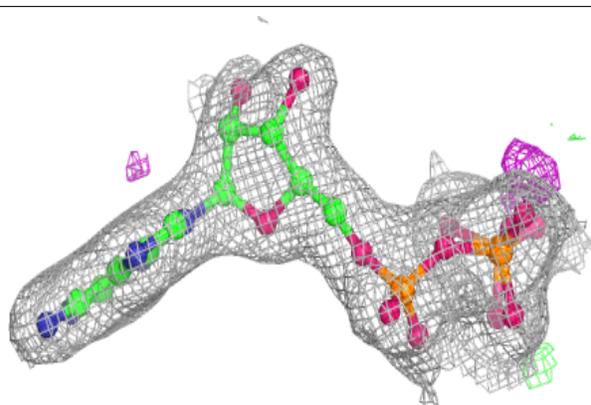
Electron density around MG A 1002:

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

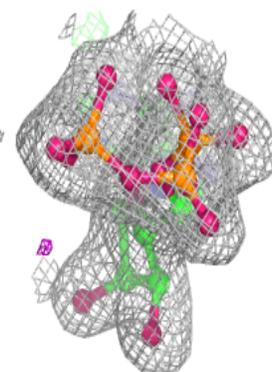
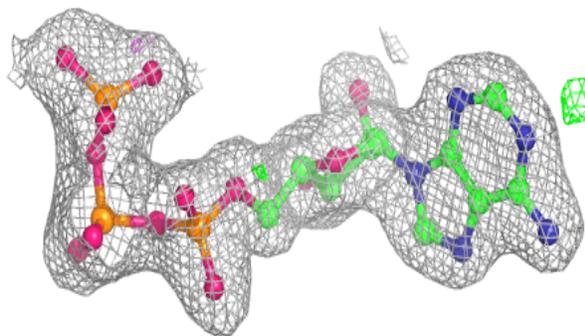
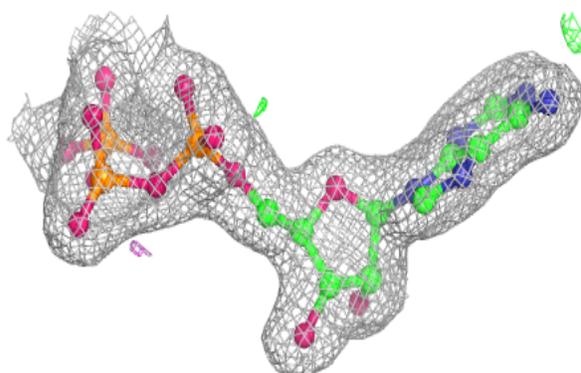


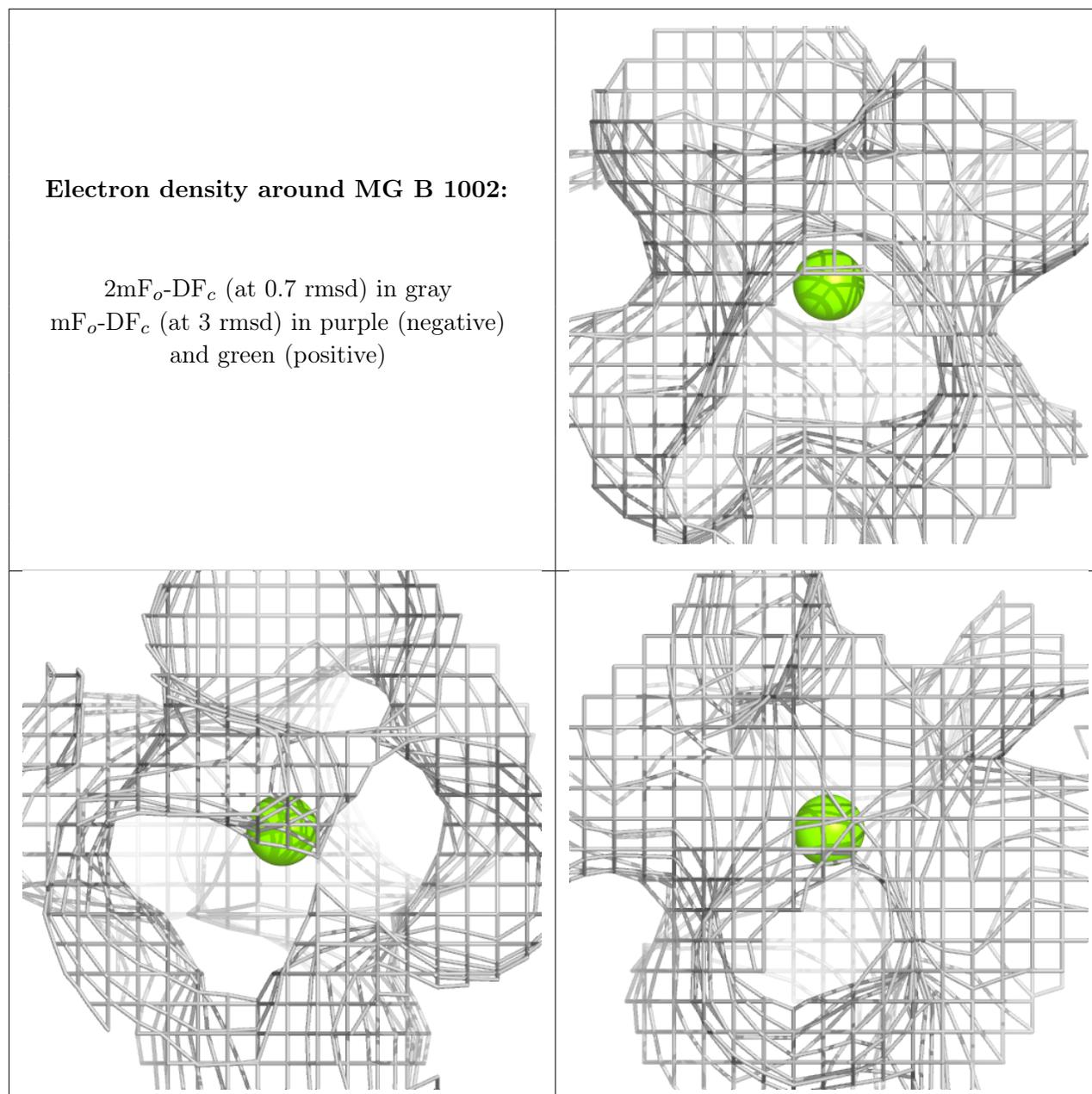
Electron density around ATP B 1001:

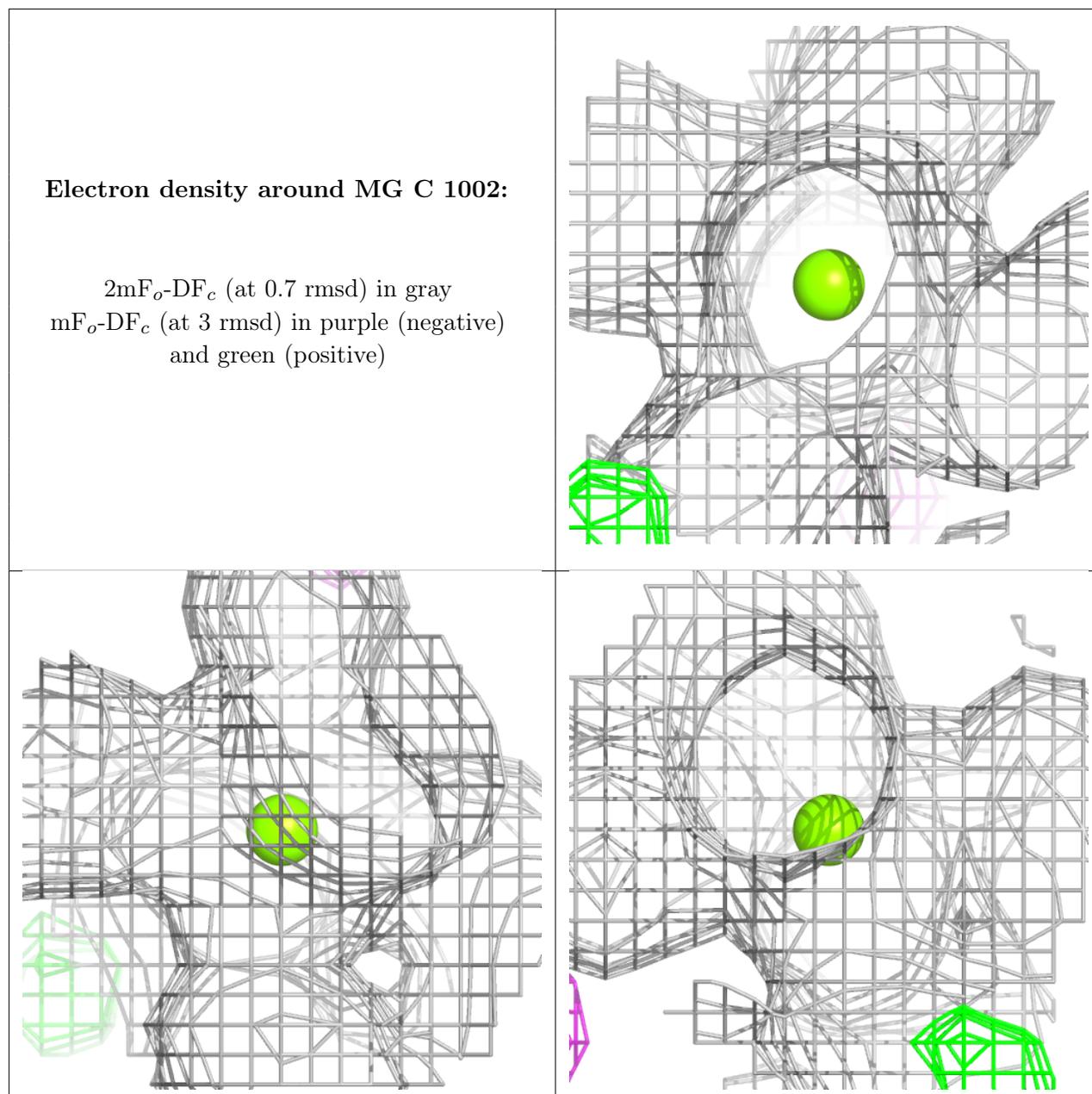
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

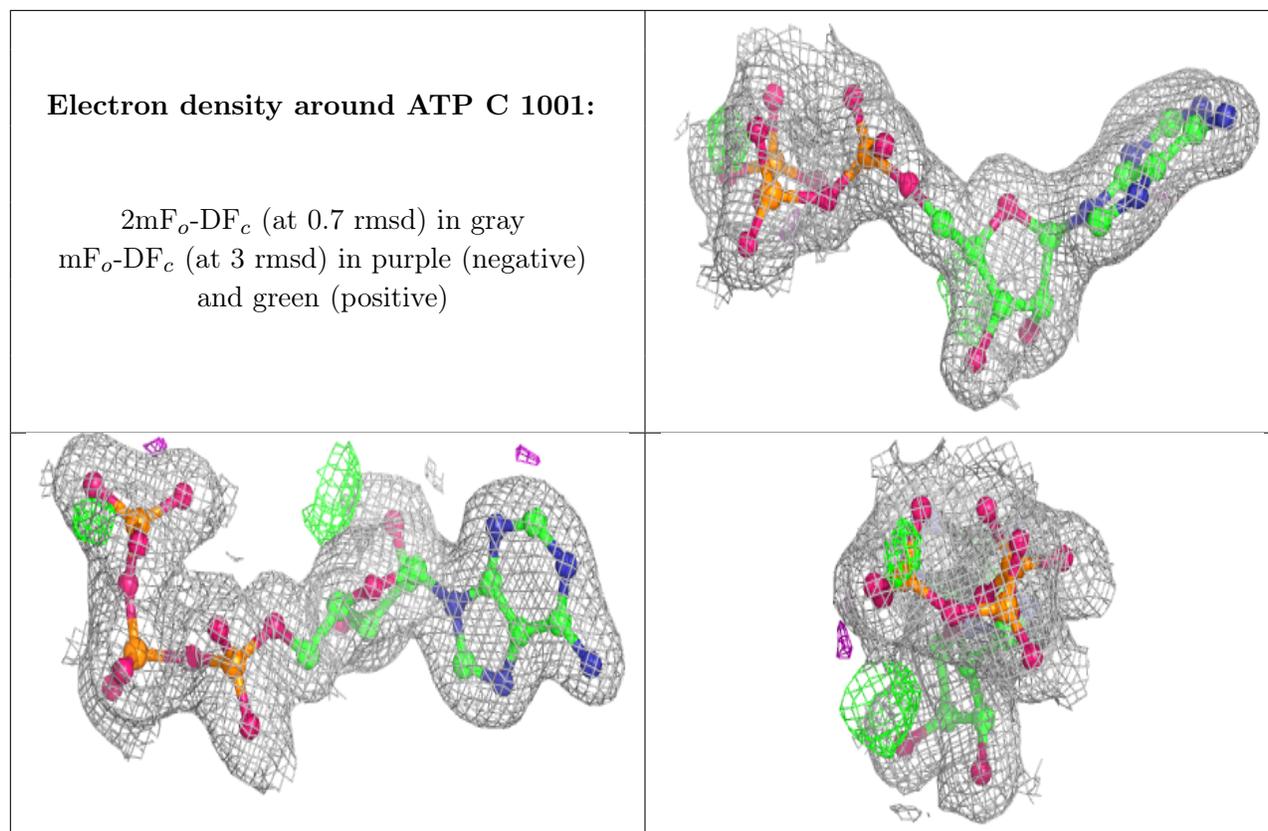
**Electron density around ATP A 1001:**

$2mF_o-DF_c$ (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.