Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 04:25 PM JST

PDB ID	:	7Y28
Title	:	Controlling fibrosis using compound with novel binding mode to prolyl-tRNA synthetase 1
Authors	:	Kim, S.; Yoon, I.; Son, J.; Park, S.; Hwang, K.Y.
Deposited on	:	2022-06-09
Resolution	:	2.29 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:

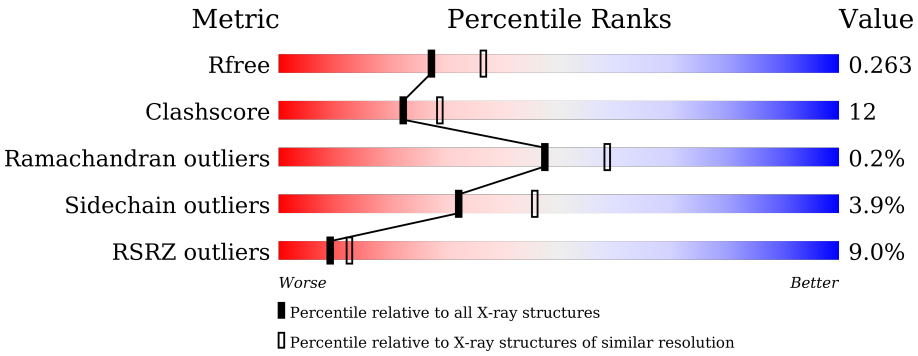
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	497	6% 78% 18%
1	B	497	11% 65% 26% 6%

2 Entry composition

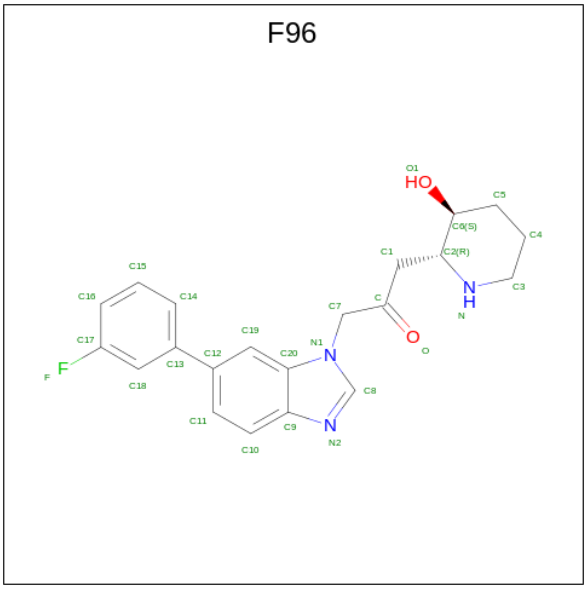
There are 6 unique types of molecules in this entry. The entry contains 7880 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional glutamate/proline--tRNA ligase.

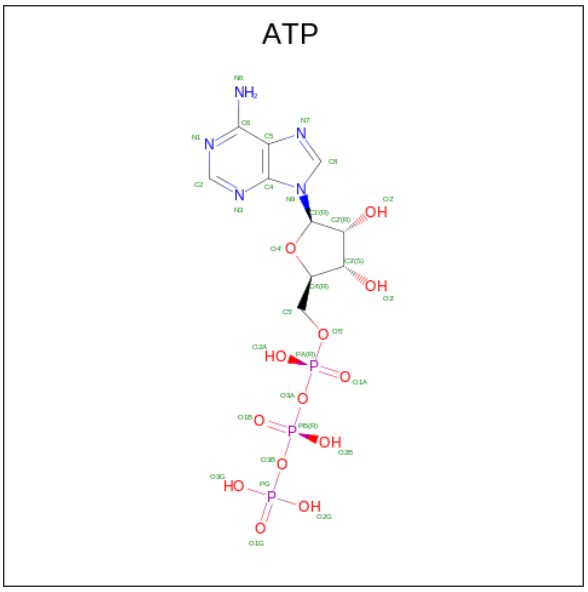
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3859	2472	652	711	24			
1	B	468	Total	C	N	O	S	0	0	0
			3767	2416	634	695	22			

- Molecule 2 is 1-[6-(3-fluorophenyl)benzimidazol-1-yl]-3-[(2R,3S)-3-oxidanylpiperidin-2-yl]propan-2-one (three-letter code: F96) (formula: $C_{21}H_{22}FN_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			27	21	1	3	2		
2	B	1	Total	C	F	N	O	0	0
			27	21	1	3	2		

- 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
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	B	2	Total	Mg	0	0
			2	2		

- Molecule 6 is water.

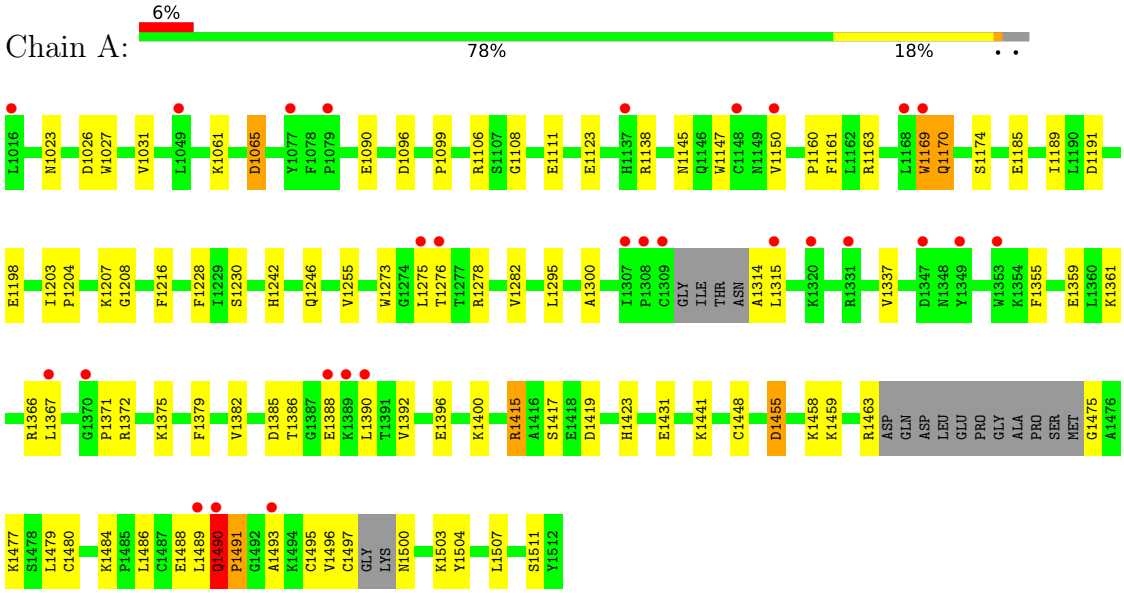
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	77	Total O 77 77	0	0
6	B	55	Total O 55 55	0	0

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.

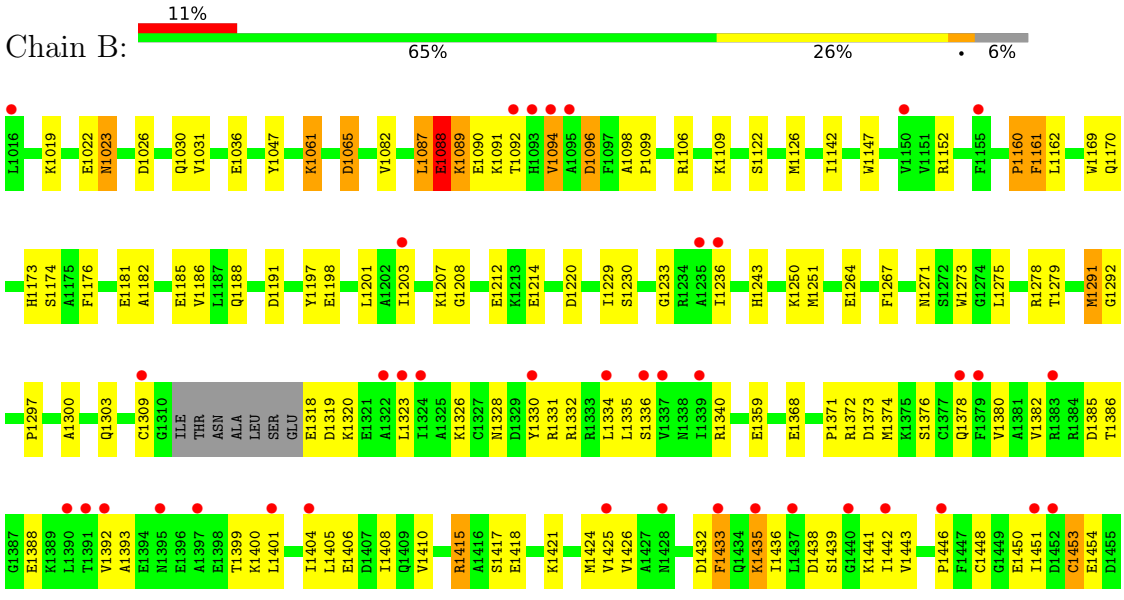
• Molecule 1: Bifunctional glutamate/proline--tRNA ligase

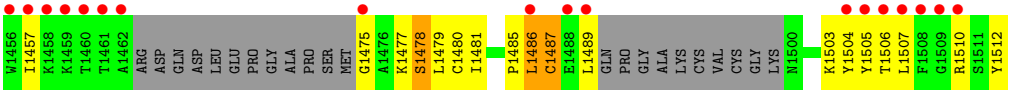
Chain A:



• Molecule 1: Bifunctional glutamate/proline--tRNA ligase

Chain B:




W1456
I1457
K1458
K1459
T1460
T1461
A1462
ARG
ASP
GLN
ASP
LEU
GLU
PRO
GLY
ALA
PRO
SER
MET
G1475
A1476
K1477
S1478
L1479
C1480
I1481
P1485
L1486
C1487
E1488
L1489
GLN
PRO
GLY
ALA
LYS
CYS
VAL
CYS
GLY
LYS
N1500
K1503
Y1504
Y1505
T1506
L1507
F1508
G1509
R1510
S1511
Y1512

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.56Å 92.38Å 86.06Å 90.00° 108.72° 90.00°	Depositor
Resolution (Å)	45.43 – 2.29 45.44 – 2.29	Depositor EDS
% Data completeness (in resolution range)	93.8 (45.43-2.29) 93.9 (45.44-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20_4438	Depositor
R, R_{free}	0.207 , 0.264 0.207 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7880	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, MG, F96, ATP

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	0.51	1/3950 (0.0%)	0.70	2/5345 (0.0%)
1	B	0.54	1/3857 (0.0%)	0.85	17/5221 (0.3%)
All	All	0.53	2/7807 (0.0%)	0.78	19/10566 (0.2%)

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	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1485	PRO	CG-CD	-7.53	1.25	1.50
1	A	1497	CYS	CB-SG	-5.20	1.73	1.81

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1486	LEU	CB-CG-CD1	-13.57	87.93	111.00
1	B	1096	ASP	CB-CG-OD2	-10.95	108.45	118.30
1	B	1485	PRO	CA-N-CD	-8.62	99.43	111.50
1	B	1486	LEU	CA-CB-CG	8.48	134.80	115.30
1	A	1160	PRO	C-N-CA	8.25	142.33	121.70
1	B	1160	PRO	C-N-CA	8.14	142.06	121.70
1	A	1490	GLN	C-N-CD	-7.77	103.51	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1087	LEU	CB-CG-CD1	-7.76	97.81	111.00
1	B	1094	VAL	C-N-CA	-7.04	104.09	121.70
1	B	1485	PRO	CA-CB-CG	-6.55	91.55	104.00
1	B	1486	LEU	N-CA-CB	-6.22	97.96	110.40
1	B	1096	ASP	CB-CG-OD1	6.06	123.75	118.30
1	B	1161	PHE	CB-CA-C	-6.02	98.36	110.40
1	B	1453	CYS	CA-CB-SG	5.84	124.51	114.00
1	B	1415	ARG	CG-CD-NE	5.59	123.55	111.80
1	B	1485	PRO	N-CD-CG	-5.35	95.18	103.20
1	B	1477	LYS	CA-CB-CG	5.27	124.99	113.40
1	B	1291	MET	CB-CG-SD	-5.17	96.91	112.40
1	B	1487	CYS	CA-CB-SG	5.11	123.19	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1315	LEU	Peptide
1	A	1490	GLN	Peptide
1	B	1088	GLU	Peptide
1	B	1330	TYR	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	3859	0	3820	62	0
1	B	3767	0	3719	117	0
2	A	27	0	0	1	0
2	B	27	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	77	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	55	0	0	9	0
All	All	7880	0	7563	179	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 12.

All (179) 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:B:1331:ARG:HG3	1:B:1332:ARG:H	1.13	1.07
1:B:1090:GLU:HG3	1:B:1091:LYS:H	1.21	1.03
1:B:1436:ILE:HA	1:B:1441:LYS:HZ3	1.27	0.96
1:B:1332:ARG:HA	1:B:1335:LEU:HB2	1.48	0.94
1:B:1331:ARG:CG	1:B:1332:ARG:H	1.83	0.90
1:A:1314:ALA:N	6:A:2702:HOH:O	2.05	0.89
1:B:1426:VAL:HG13	1:B:1486:LEU:HD11	1.54	0.89
1:B:1300:ALA:O	1:B:1340:ARG:NH1	2.07	0.88
1:B:1090:GLU:CG	1:B:1091:LYS:H	1.89	0.86
1:B:1442:ILE:HD12	1:B:1507:LEU:HD11	1.59	0.85
1:B:1331:ARG:HG3	1:B:1332:ARG:N	1.92	0.84
1:B:1328:ASN:O	1:B:1331:ARG:HB2	1.80	0.80
1:A:1463:ARG:O	6:A:2701:HOH:O	2.00	0.79
1:A:1459:LYS:O	1:A:1459:LYS:HD2	1.84	0.78
1:B:1475:GLY:N	6:B:2705:HOH:O	2.19	0.74
1:A:1495:CYS:SG	1:A:1496:VAL:N	2.61	0.74
1:A:1023:ASN:ND2	1:A:1026:ASP:OD1	2.19	0.74
1:A:1191:ASP:OD1	1:A:1207:LYS:NZ	2.20	0.73
1:B:1090:GLU:HG3	1:B:1091:LYS:N	2.01	0.73
1:B:1426:VAL:CG1	1:B:1486:LEU:HD11	2.19	0.73
1:B:1332:ARG:O	1:B:1336:SER:N	2.11	0.73
1:B:1122:SER:HB2	1:B:1126:MET:HE2	1.70	0.72
1:A:1390:LEU:HD22	1:A:1392:VAL:HG22	1.72	0.72
1:A:1459:LYS:NZ	6:A:2705:HOH:O	2.23	0.72
1:B:1439:SER:OG	1:B:1441:LYS:NZ	2.18	0.71
1:B:1436:ILE:HB	1:B:1441:LYS:HE2	1.72	0.71
1:B:1436:ILE:HD11	1:B:1443:VAL:HB	1.72	0.69
1:B:1475:GLY:N	6:B:2709:HOH:O	2.25	0.69
1:B:1094:VAL:O	1:B:1096:ASP:N	2.25	0.69
1:A:1490:GLN:HA	1:A:1493:ALA:H	1.58	0.69
1:A:1161:PHE:O	1:A:1278:ARG:HA	1.94	0.68
1:B:1188:GLN:OE1	6:B:2702:HOH:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1489:LEU:HG	1:A:1490:GLN:HB3	1.77	0.65
1:A:1145:ASN:OD1	1:A:1170:GLN:HG2	1.96	0.65
1:B:1036:GLU:O	6:B:2701:HOH:O	2.13	0.65
1:B:1264:GLU:OE2	6:B:2703:HOH:O	2.14	0.65
1:B:1318:GLU:HG2	1:B:1319:ASP:H	1.61	0.65
1:B:1297:PRO:HG2	1:B:1408:ILE:HG23	1.77	0.64
1:B:1191:ASP:OD1	1:B:1207:LYS:NZ	2.29	0.64
1:B:1291:MET:HE1	1:B:1359:GLU:OE1	1.98	0.63
1:B:1406:GLU:O	1:B:1410:VAL:HG23	2.01	0.61
1:B:1454:GLU:HA	1:B:1457:ILE:HD12	1.83	0.61
1:B:1400:LYS:O	1:B:1404:ILE:HD12	2.00	0.60
1:A:1096:ASP:O	1:A:1099:PRO:HD2	2.01	0.60
1:A:1246:GLN:OE1	6:A:2703:HOH:O	2.15	0.60
1:A:1230:SER:OG	1:A:1419:ASP:OD2	2.15	0.60
1:B:1332:ARG:O	1:B:1336:SER:OG	2.20	0.59
1:B:1122:SER:HB2	1:B:1126:MET:CE	2.31	0.59
1:B:1450:GLU:OE2	6:B:2704:HOH:O	2.16	0.59
1:A:1203:ILE:HD13	1:A:1282:VAL:HG12	1.84	0.59
1:A:1366:ARG:CZ	1:A:1382:VAL:HG11	2.32	0.59
1:B:1446:PRO:HD3	1:B:1505:TYR:CE2	2.37	0.59
1:A:1090:GLU:O	6:A:2704:HOH:O	2.16	0.58
1:B:1368:GLU:HB2	1:B:1380:VAL:HG12	1.85	0.58
1:A:1216:PHE:HB2	1:A:1242:HIS:CE1	2.39	0.58
1:B:1432:ASP:O	1:B:1436:ILE:HG23	2.03	0.58
1:B:1236:ILE:HG13	1:B:1512:TYR:HB2	1.85	0.57
1:B:1481:ILE:HG12	1:B:1506:THR:HG22	1.86	0.57
1:A:1400:LYS:O	1:A:1400:LYS:HD3	2.03	0.57
1:A:1106:ARG:NH1	1:A:1108:GLY:O	2.36	0.57
1:A:1061:LYS:O	1:A:1065:ASP:HB2	2.04	0.57
1:B:1418:GLU:HA	1:B:1421:LYS:HG2	1.86	0.57
1:A:1479:LEU:HD12	1:A:1507:LEU:HG	1.87	0.56
1:B:1479:LEU:HD12	1:B:1507:LEU:HG	1.87	0.56
1:B:1510:ARG:NH1	6:B:2709:HOH:O	2.30	0.56
1:B:1368:GLU:HB2	1:B:1380:VAL:CG1	2.35	0.56
1:B:1454:GLU:OE2	1:B:1478:SER:HB3	2.06	0.56
1:A:1361:LYS:NZ	6:A:2711:HOH:O	2.32	0.56
1:B:1405:LEU:HA	1:B:1408:ILE:HG22	1.88	0.55
1:B:1061:LYS:O	1:B:1065:ASP:HB2	2.07	0.55
1:B:1090:GLU:CG	1:B:1091:LYS:N	2.62	0.55
1:B:1486:LEU:HD23	1:B:1487:CYS:HB2	1.89	0.55
1:B:1303:GLN:HG3	1:B:1340:ARG:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1174:SER:OG	1:B:1185:GLU:OE1	2.24	0.54
1:B:1432:ASP:HA	1:B:1435:LYS:HB3	1.88	0.54
1:A:1477:LYS:HD3	1:A:1511:SER:OG	2.08	0.54
1:A:1198:GLU:HG2	1:A:1203:ILE:O	2.08	0.53
1:B:1436:ILE:HD11	1:B:1443:VAL:CB	2.37	0.53
1:A:1367:LEU:HD11	1:A:1379:PHE:CE2	2.43	0.53
1:A:1390:LEU:CD2	1:A:1392:VAL:HG22	2.39	0.53
1:A:1500:ASN:N	1:A:1500:ASN:HD22	2.06	0.53
1:B:1309:CYS:O	1:B:1371:PRO:HD3	2.09	0.53
1:A:1123:GLU:OE2	2:A:2601:F96:N	2.42	0.52
1:B:1082:VAL:HB	1:B:1087:LEU:HD11	1.90	0.52
1:B:1334:LEU:HD21	1:B:1401:LEU:HD12	1.91	0.52
1:B:1436:ILE:CA	1:B:1441:LYS:HZ3	2.11	0.52
1:B:1019:LYS:HB2	1:B:1022:GLU:CG	2.41	0.51
1:B:1438:ASP:OD1	1:B:1510:ARG:NH2	2.43	0.51
1:A:1174:SER:OG	1:A:1185:GLU:OE1	2.29	0.51
1:A:1475:GLY:N	6:A:2719:HOH:O	2.44	0.51
1:A:1448:CYS:O	1:A:1503:LYS:HG3	2.11	0.50
1:A:1489:LEU:HG	1:A:1490:GLN:N	2.26	0.50
1:B:1332:ARG:HG3	1:B:1335:LEU:HB2	1.94	0.50
1:B:1392:VAL:HG12	1:B:1393:ALA:O	2.11	0.50
1:B:1453:CYS:O	1:B:1457:ILE:HD12	2.12	0.49
1:B:1373:ASP:HB3	1:B:1378:GLN:O	2.13	0.49
1:B:1176:PHE:CD2	1:B:1181:GLU:HB3	2.47	0.49
1:B:1122:SER:CB	1:B:1126:MET:HE2	2.39	0.49
1:B:1208:GLY:HA3	1:B:1480:CYS:SG	2.52	0.49
1:A:1366:ARG:HB3	1:A:1382:VAL:HG13	1.95	0.48
1:B:1106:ARG:NE	6:B:2714:HOH:O	2.39	0.48
1:A:1371:PRO:O	1:A:1375:LYS:HG3	2.14	0.48
1:A:1295:LEU:HD13	1:A:1300:ALA:HA	1.96	0.48
1:B:1109:LYS:HA	1:B:1109:LYS:HD2	1.61	0.48
1:B:1090:GLU:HB3	1:B:1251:MET:CG	2.44	0.48
1:B:1126:MET:HE3	1:B:1173:HIS:CE1	2.48	0.48
1:B:1405:LEU:HA	1:B:1408:ILE:CG2	2.43	0.48
1:B:1385:ASP:OD1	1:B:1386:THR:N	2.47	0.48
1:B:1448:CYS:O	1:B:1503:LYS:HE2	2.13	0.48
1:A:1150:VAL:HG21	1:A:1169:TRP:CE2	2.49	0.47
1:A:1392:VAL:HG12	1:A:1396:GLU:HG3	1.97	0.47
1:A:1423:HIS:HA	1:A:1441:LYS:HG2	1.97	0.47
1:B:1229:ILE:HD12	1:B:1512:TYR:HE2	1.80	0.47
1:B:1451:ILE:O	1:B:1454:GLU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1486:LEU:HD23	1:B:1487:CYS:CB	2.45	0.46
1:A:1106:ARG:HB3	1:A:1111:GLU:HA	1.97	0.46
1:B:1152:ARG:NH1	3:B:2602:ATP:O1A	2.43	0.46
1:B:1230:SER:O	1:B:1233:GLY:N	2.45	0.46
1:B:1399:THR:HG23	6:B:2730:HOH:O	2.15	0.46
1:A:1458:LYS:HD2	1:A:1475:GLY:HA3	1.97	0.46
1:B:1096:ASP:O	1:B:1099:PRO:HD2	2.15	0.46
1:B:1323:LEU:HA	1:B:1374:MET:SD	2.55	0.46
1:B:1229:ILE:HD12	1:B:1512:TYR:CE2	2.50	0.46
1:B:1454:GLU:HA	1:B:1457:ILE:CD1	2.45	0.46
1:B:1489:LEU:HB2	1:B:1505:TYR:CD1	2.51	0.46
1:B:1026:ASP:O	1:B:1030:GLN:HG2	2.16	0.46
1:A:1027:TRP:CE2	1:A:1031:VAL:HG21	2.51	0.45
1:A:1379:PHE:CZ	1:A:1392:VAL:HB	2.52	0.45
1:A:1169:TRP:CB	1:A:1276:THR:HG22	2.46	0.45
1:A:1455:ASP:N	1:A:1455:ASP:OD1	2.49	0.45
1:A:1208:GLY:HA3	1:A:1480:CYS:SG	2.57	0.45
1:B:1170:GLN:HE21	1:B:1275:LEU:HB3	1.81	0.45
1:A:1490:GLN:HA	1:A:1493:ALA:CB	2.47	0.44
1:B:1404:ILE:O	1:B:1408:ILE:HG22	2.16	0.44
1:A:1388:GLU:HA	1:A:1388:GLU:OE1	2.17	0.44
1:B:1186:VAL:HG21	1:B:1243:HIS:HB2	1.98	0.44
1:A:1415:ARG:O	1:A:1415:ARG:HD3	2.17	0.44
1:B:1161:PHE:O	1:B:1278:ARG:HA	2.17	0.44
1:B:1061:LYS:HG3	1:B:1147:TRP:CZ2	2.53	0.44
1:A:1295:LEU:HB3	1:A:1300:ALA:HB2	1.99	0.44
1:A:1490:GLN:HG3	1:A:1491:PRO:N	2.32	0.44
1:B:1088:GLU:OE2	1:B:1089:LYS:HA	2.17	0.44
1:B:1198:GLU:HG2	1:B:1203:ILE:O	2.18	0.44
1:B:1197:TYR:CZ	1:B:1279:THR:HG22	2.53	0.43
1:A:1385:ASP:OD1	1:A:1386:THR:N	2.51	0.43
1:A:1147:TRP:CE3	1:A:1170:GLN:HB2	2.54	0.43
1:B:1201:LEU:O	1:B:1203:ILE:HG13	2.18	0.43
1:B:1098:ALA:N	1:B:1099:PRO:CD	2.82	0.43
1:B:1023:ASN:OD1	1:B:1026:ASP:OD2	2.36	0.43
1:B:1433:PHE:HD2	1:B:1443:VAL:HG11	1.83	0.43
1:B:1182:ALA:O	1:B:1271:ASN:ND2	2.44	0.43
1:B:1147:TRP:CE3	1:B:1170:GLN:HB3	2.52	0.43
1:B:1426:VAL:HG22	1:B:1486:LEU:CD1	2.48	0.43
1:B:1448:CYS:O	1:B:1503:LYS:HG3	2.19	0.43
1:B:1142:ILE:O	1:B:1174:SER:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1019:LYS:HB2	1:B:1022:GLU:HG2	2.00	0.42
1:B:1212:GLU:HG2	1:B:1451:ILE:HD11	2.00	0.42
1:B:1425:VAL:O	1:B:1443:VAL:HG23	2.19	0.42
1:A:1511:SER:N	6:A:2706:HOH:O	2.24	0.42
1:B:1031:VAL:HG22	1:B:1292:GLY:HA2	2.00	0.42
1:A:1189:ILE:HD13	1:A:1189:ILE:HA	1.83	0.42
1:B:1047:TYR:CE1	1:B:1160:PRO:HG3	2.55	0.42
1:B:1250:LYS:HA	1:B:1267:PHE:CE1	2.55	0.42
1:B:1160:PRO:C	1:B:1162:LEU:H	2.23	0.41
1:A:1355:PHE:O	1:A:1359:GLU:HG3	2.21	0.41
1:B:1424:MET:HA	1:B:1442:ILE:O	2.20	0.41
1:B:1426:VAL:HG22	1:B:1486:LEU:HD12	2.02	0.41
1:B:1475:GLY:N	1:B:1510:ARG:NH1	2.69	0.41
1:A:1204:PRO:HG3	1:A:1417:SER:HA	2.01	0.41
1:A:1228:PHE:CE2	1:A:1230:SER:HA	2.57	0.40
1:A:1458:LYS:O	1:A:1475:GLY:HA3	2.21	0.40
1:B:1082:VAL:HB	1:B:1087:LEU:CD1	2.51	0.40
1:B:1382:VAL:HA	1:B:1388:GLU:O	2.22	0.40
1:B:1417:SER:O	1:B:1421:LYS:HG2	2.21	0.40
1:A:1169:TRP:HB3	1:A:1276:THR:HG22	2.03	0.40
1:B:1320:LYS:O	1:B:1323:LEU:N	2.52	0.40
1:A:1486:LEU:HD23	1:A:1486:LEU:HA	1.93	0.40
1:B:1214:GLU:HA	1:B:1214:GLU:OE1	2.22	0.40
1:B:1326:LYS:HB2	1:B:1326:LYS:HE2	1.94	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	472/497 (95%)	463 (98%)	7 (2%)	2 (0%)	34 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	460/497 (93%)	446 (97%)	14 (3%)	0	100 100
All	All	932/994 (94%)	909 (98%)	21 (2%)	2 (0%)	47 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1490	GLN
1	A	1491	PRO

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	415/428 (97%)	399 (96%)	16 (4%)	32 46
1	B	404/428 (94%)	388 (96%)	16 (4%)	31 44
All	All	819/856 (96%)	787 (96%)	32 (4%)	32 46

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1065	ASP
1	A	1138	ARG
1	A	1163	ARG
1	A	1169	TRP
1	A	1170	GLN
1	A	1255	VAL
1	A	1273	TRP
1	A	1275	LEU
1	A	1337	VAL
1	A	1372	ARG
1	A	1415	ARG
1	A	1431	GLU
1	A	1455	ASP
1	A	1484	LYS

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Mol	Chain	Res	Type
1	A	1488	GLU
1	A	1504	TYR
1	B	1023	ASN
1	B	1061	LYS
1	B	1065	ASP
1	B	1088	GLU
1	B	1089	LYS
1	B	1092	THR
1	B	1169	TRP
1	B	1220	ASP
1	B	1273	TRP
1	B	1372	ARG
1	B	1376	SER
1	B	1415	ARG
1	B	1433	PHE
1	B	1435	LYS
1	B	1478	SER
1	B	1504	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1378	GLN
1	B	1023	ASN
1	B	1093	HIS
1	B	1170	GLN
1	B	1266	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 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	F96	A	2601	-	29,30,30	0.72	1 (3%)	31,42,42	0.95	2 (6%)
2	F96	B	2601	-	29,30,30	0.61	0	31,42,42	1.54	2 (6%)
3	ATP	A	2602	5	26,33,33	0.51	0	31,52,52	0.86	2 (6%)
3	ATP	B	2602	5	26,33,33	0.55	0	31,52,52	0.99	1 (3%)

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	F96	A	2601	-	-	0/12/23/23	0/4/4/4
2	F96	B	2601	-	-	1/12/23/23	0/4/4/4
3	ATP	A	2602	5	-	5/18/38/38	0/3/3/3
3	ATP	B	2602	5	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2601	F96	C6-C2	2.13	1.54	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2601	F96	C5-C6-C2	-7.24	106.16	110.89
3	B	2602	ATP	C3'-C2'-C1'	3.04	105.56	100.98
2	A	2601	F96	C12-C19-C20	-2.90	118.77	121.87
2	B	2601	F96	C12-C19-C20	-2.74	118.94	121.87
2	A	2601	F96	C19-C20-C9	2.26	122.78	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2602	ATP	C5-C6-N6	2.26	123.78	120.35
3	A	2602	ATP	C3'-C2'-C1'	2.11	104.15	100.98

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2602	ATP	C5'-O5'-PA-O2A
3	B	2602	ATP	C5'-O5'-PA-O2A
3	B	2602	ATP	C5'-O5'-PA-O3A
3	B	2602	ATP	O4'-C4'-C5'-O5'
3	B	2602	ATP	C3'-C4'-C5'-O5'
3	A	2602	ATP	C5'-O5'-PA-O3A
3	A	2602	ATP	C5'-O5'-PA-O1A
2	B	2601	F96	O-C-C7-N1
3	A	2602	ATP	C4'-C5'-O5'-PA
3	A	2602	ATP	O4'-C4'-C5'-O5'

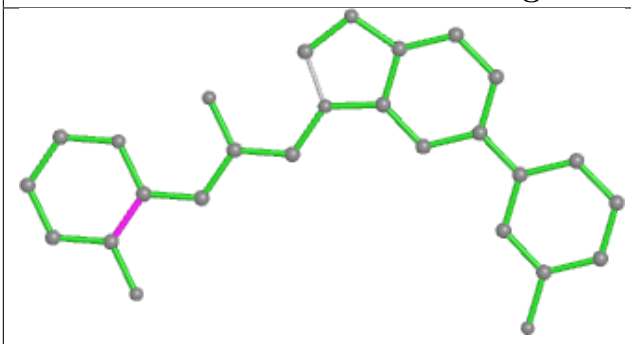
There are no ring outliers.

2 monomers are involved in 2 short contacts:

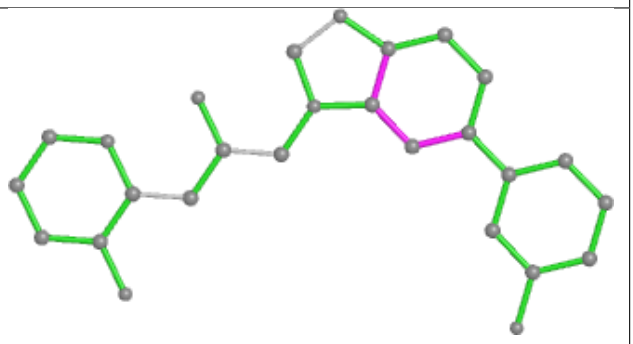
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2601	F96	1	0
3	B	2602	ATP	1	0

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 then 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.

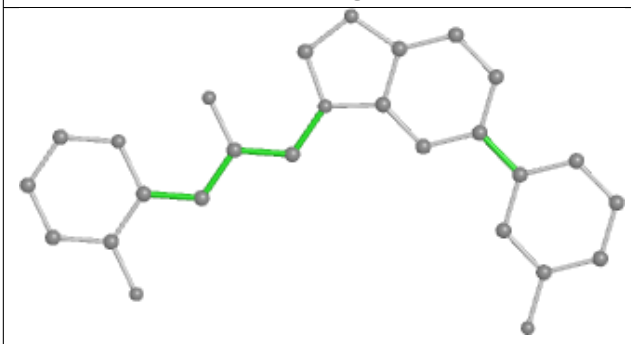
Ligand F96 A 2601



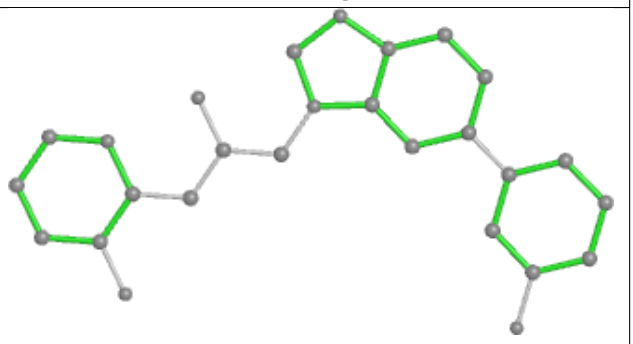
Bond lengths



Bond angles

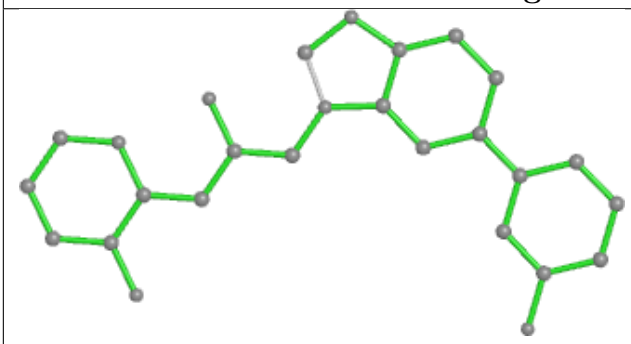


Torsions

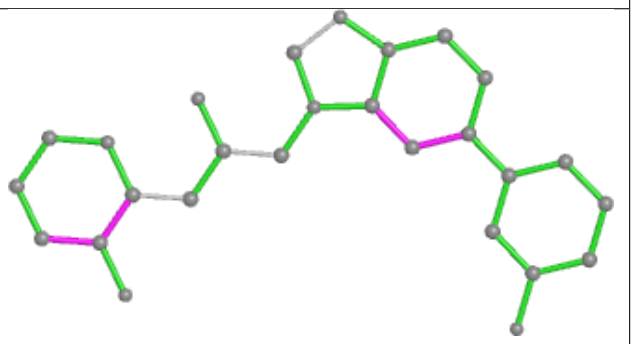


Rings

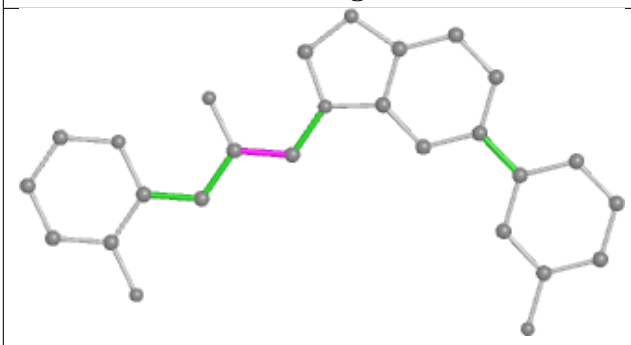
Ligand F96 B 2601



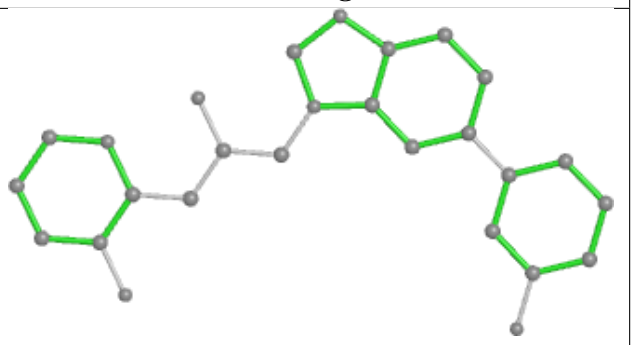
Bond lengths



Bond angles

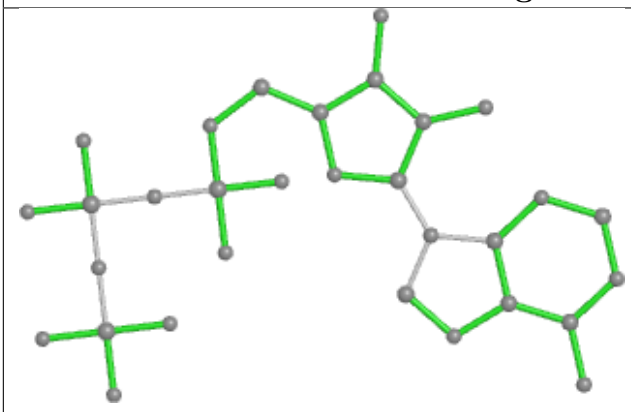


Torsions

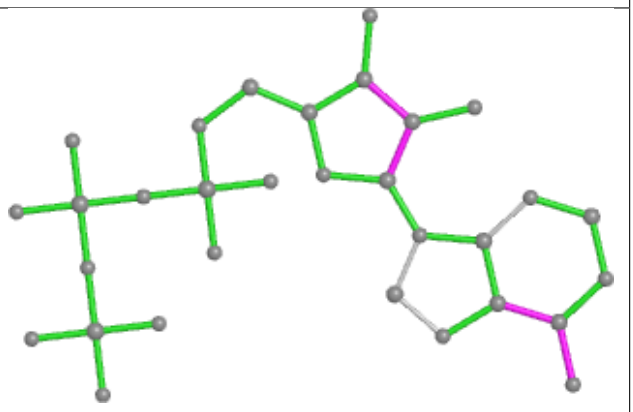


Rings

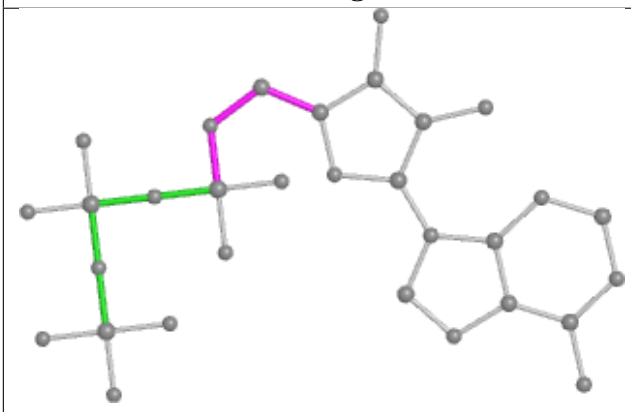
Ligand ATP A 2602



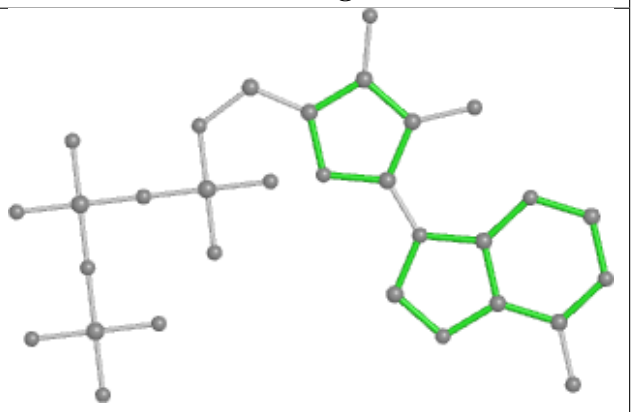
Bond lengths



Bond angles

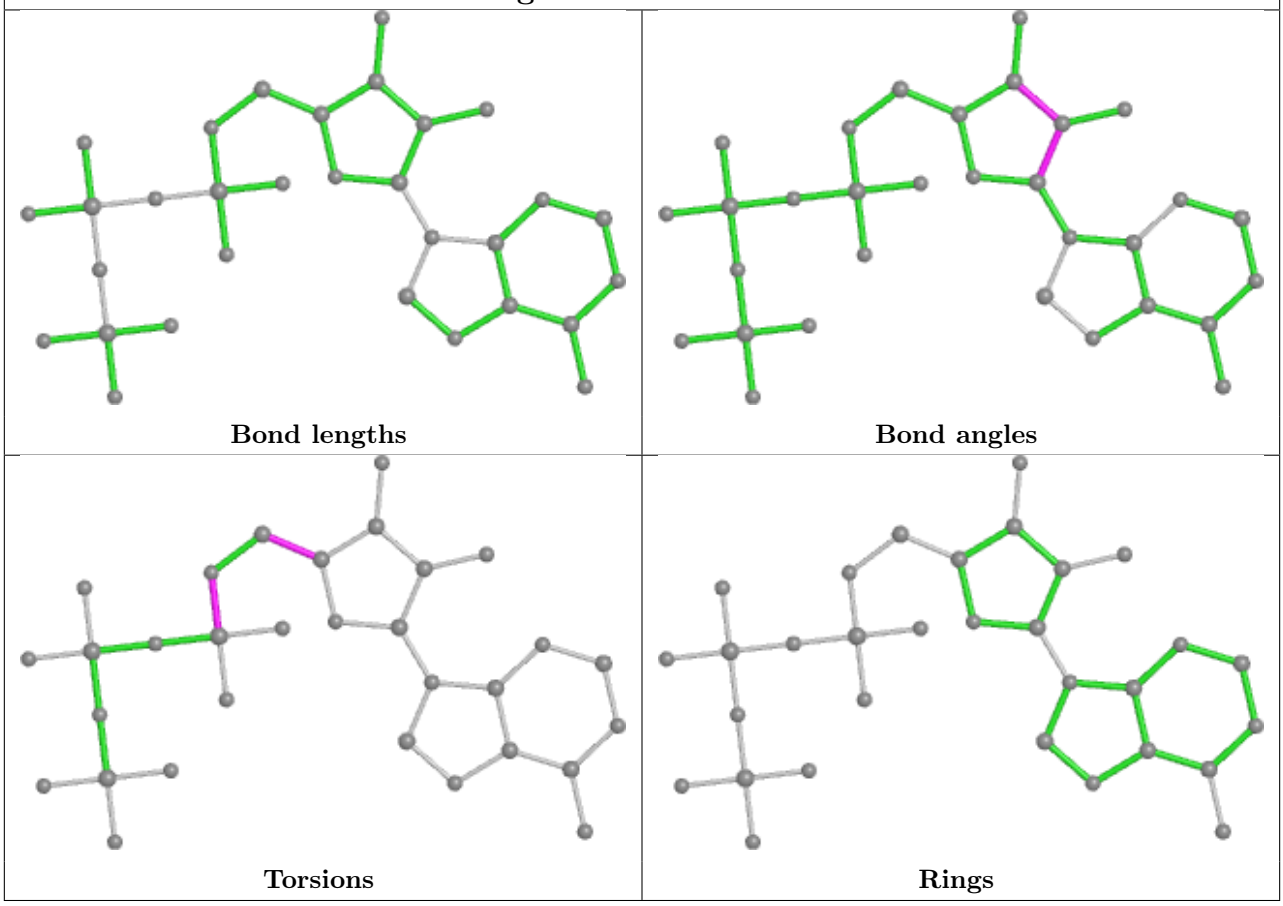


Torsions



Rings

Ligand ATP B 2602



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^{th} 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	480/497 (96%)	0.41	28 (5%) 23 29	21, 46, 71, 96	0
1	B	468/497 (94%)	0.76	57 (12%) 4 6	24, 54, 92, 110	0
All	All	948/994 (95%)	0.58	85 (8%) 9 12	21, 49, 87, 110	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1092	THR	8.8
1	B	1155	PHE	8.4
1	B	1433	PHE	7.7
1	A	1347	ASP	5.2
1	B	1397	ALA	4.9
1	B	1462	ALA	4.7
1	B	1093	HIS	4.7
1	B	1486	LEU	4.7
1	B	1401	LEU	4.6
1	B	1461	THR	4.6
1	B	1095	ALA	4.5
1	B	1435	LYS	4.5
1	B	1425	VAL	4.4
1	B	1442	ILE	4.4
1	A	1370	GLY	4.4
1	B	1390	LEU	4.3
1	B	1395	ASN	4.1
1	B	1094	VAL	4.0
1	B	1437	LEU	3.9
1	A	1490	GLN	3.7
1	B	1504	TYR	3.7
1	B	1391	THR	3.5
1	B	1460	THR	3.4
1	A	1309	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1392	VAL	3.4
1	A	1349	TYR	3.4
1	B	1458	LYS	3.2
1	A	1489	LEU	3.2
1	B	1475	GLY	3.2
1	B	1489	LEU	3.2
1	B	1508	PHE	3.1
1	A	1016	LEU	3.1
1	B	1323	LEU	3.1
1	A	1315	LEU	2.9
1	B	1379	PHE	2.8
1	A	1353	TRP	2.8
1	A	1390	LEU	2.7
1	A	1389	LYS	2.7
1	B	1236	ILE	2.7
1	B	1324	ILE	2.7
1	B	1235	ALA	2.7
1	B	1330	TYR	2.6
1	A	1388	GLU	2.6
1	B	1404	ILE	2.6
1	B	1510	ARG	2.6
1	A	1367	LEU	2.6
1	B	1457	ILE	2.5
1	B	1203	ILE	2.5
1	B	1507	LEU	2.4
1	B	1337	VAL	2.4
1	B	1334	LEU	2.4
1	B	1446	PRO	2.4
1	A	1137	HIS	2.3
1	A	1331	ARG	2.3
1	B	1505	TYR	2.3
1	B	1339	ILE	2.3
1	B	1336	SER	2.3
1	A	1169	TRP	2.3
1	B	1452	ASP	2.3
1	A	1077	TYR	2.3
1	A	1148	CYS	2.3
1	A	1049	LEU	2.2
1	A	1493	ALA	2.2
1	A	1276	THR	2.2
1	B	1016	LEU	2.2
1	B	1459	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1150	VAL	2.2
1	A	1307	ILE	2.2
1	B	1322	ALA	2.2
1	B	1451	ILE	2.2
1	A	1079	PRO	2.1
1	A	1275	LEU	2.1
1	B	1509	GLY	2.1
1	A	1320	LYS	2.1
1	B	1428	ASN	2.1
1	A	1168	LEU	2.1
1	B	1383	ARG	2.1
1	A	1150	VAL	2.1
1	A	1308	PRO	2.1
1	B	1506	THR	2.1
1	B	1456	TRP	2.1
1	B	1440	GLY	2.0
1	B	1378	GLN	2.0
1	B	1488	GLU	2.0
1	B	1309	CYS	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^{th} 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^2)	Q<0.9
4	ZN	B	2603	1/1	0.56	0.14	109,109,109,109	0
5	MG	B	2605	1/1	0.72	0.33	82,82,82,82	0
5	MG	B	2604	1/1	0.84	0.32	72,72,72,72	0
3	ATP	B	2602	31/31	0.85	0.17	54,67,126,133	0

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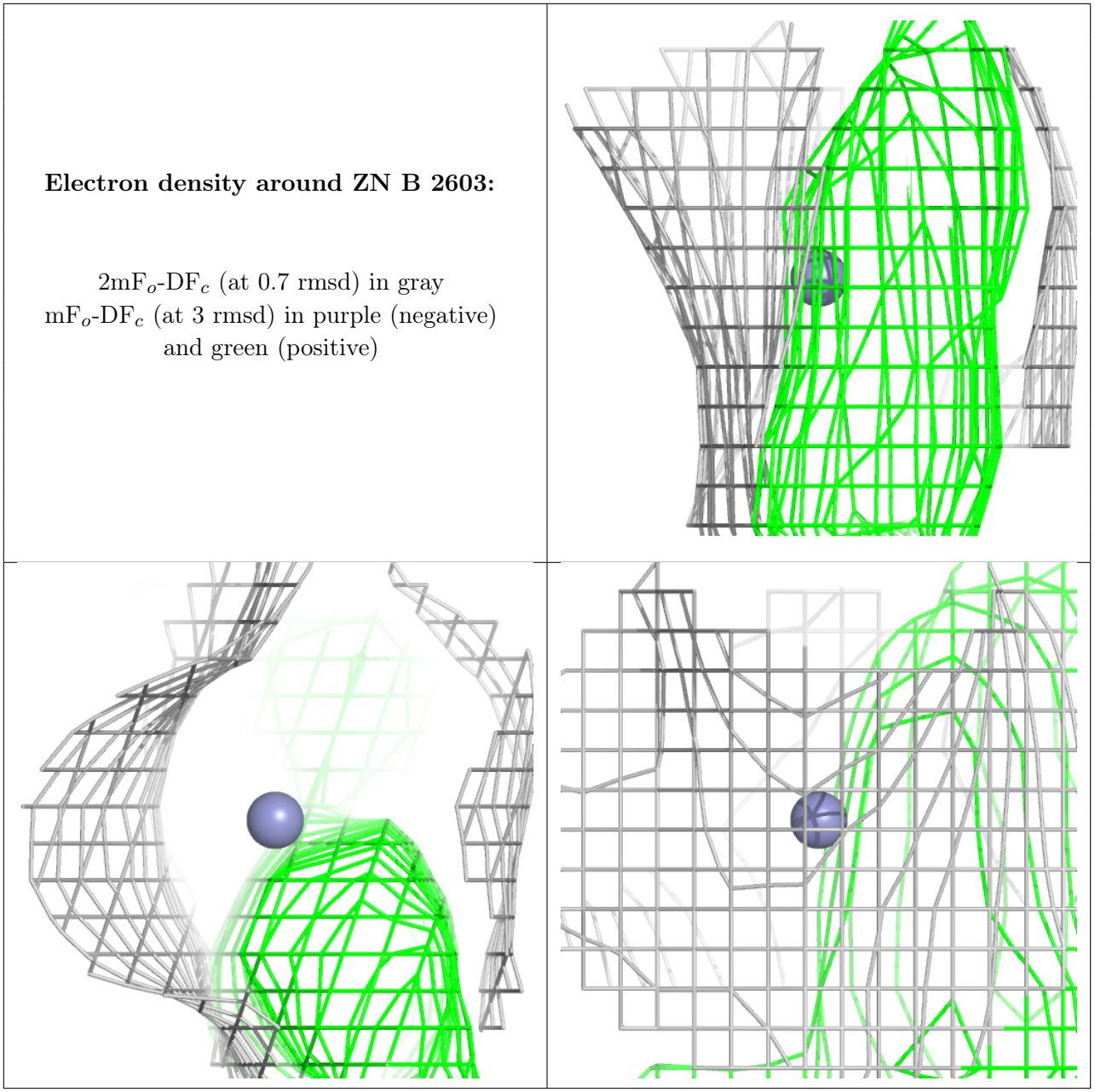
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	F96	B	2601	27/27	0.94	0.19	23,42,58,83	0
2	F96	A	2601	27/27	0.95	0.17	24,32,39,43	0
5	MG	A	2605	1/1	0.97	0.35	34,34,34,34	0
3	ATP	A	2602	31/31	0.97	0.16	25,36,46,54	0
5	MG	A	2604	1/1	0.97	0.30	29,29,29,29	0
4	ZN	A	2603	1/1	0.98	0.07	64,64,64,64	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.

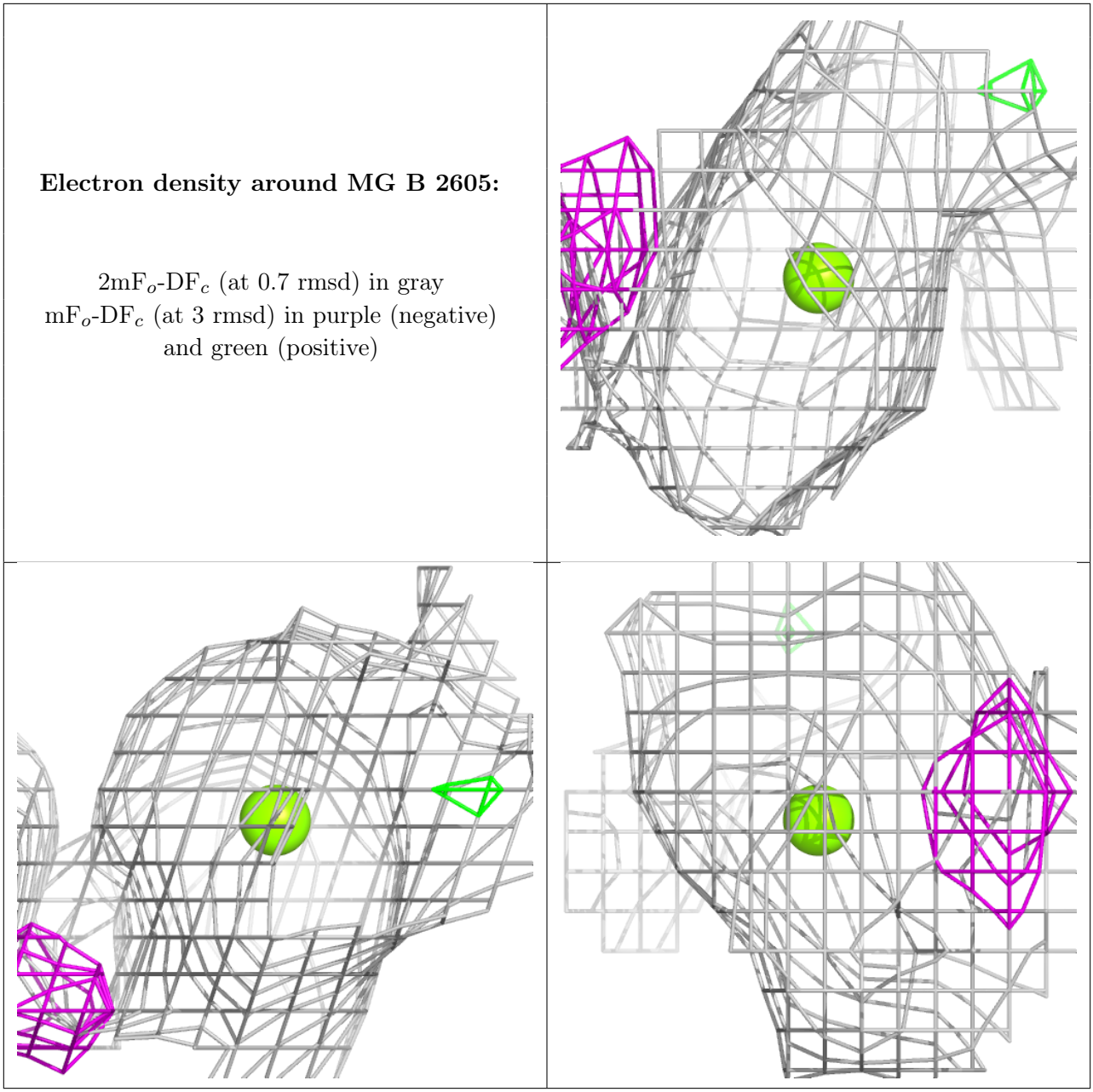
Electron density around ZN B 2603:

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



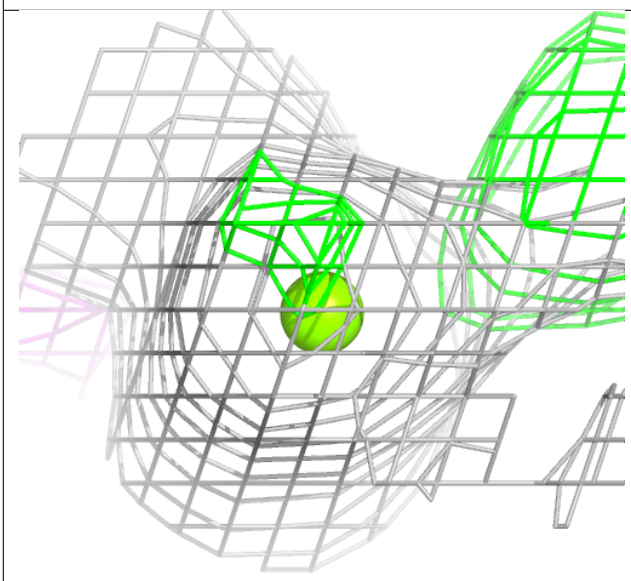
Electron density around MG B 2605:

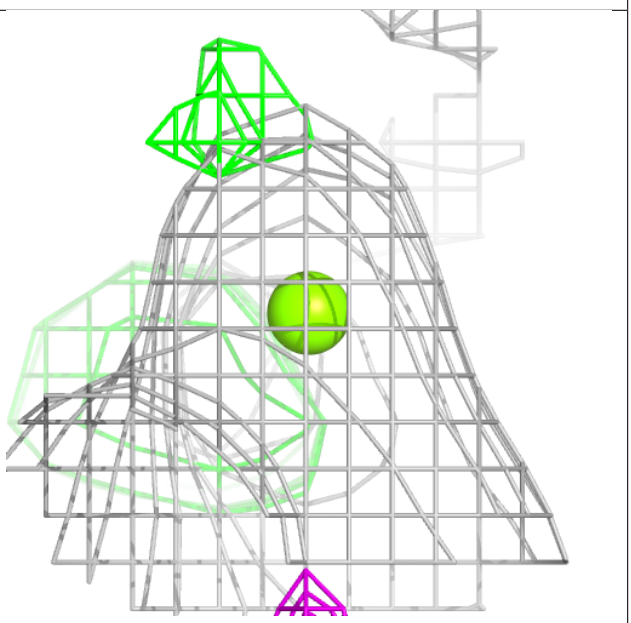
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MG B 2604:

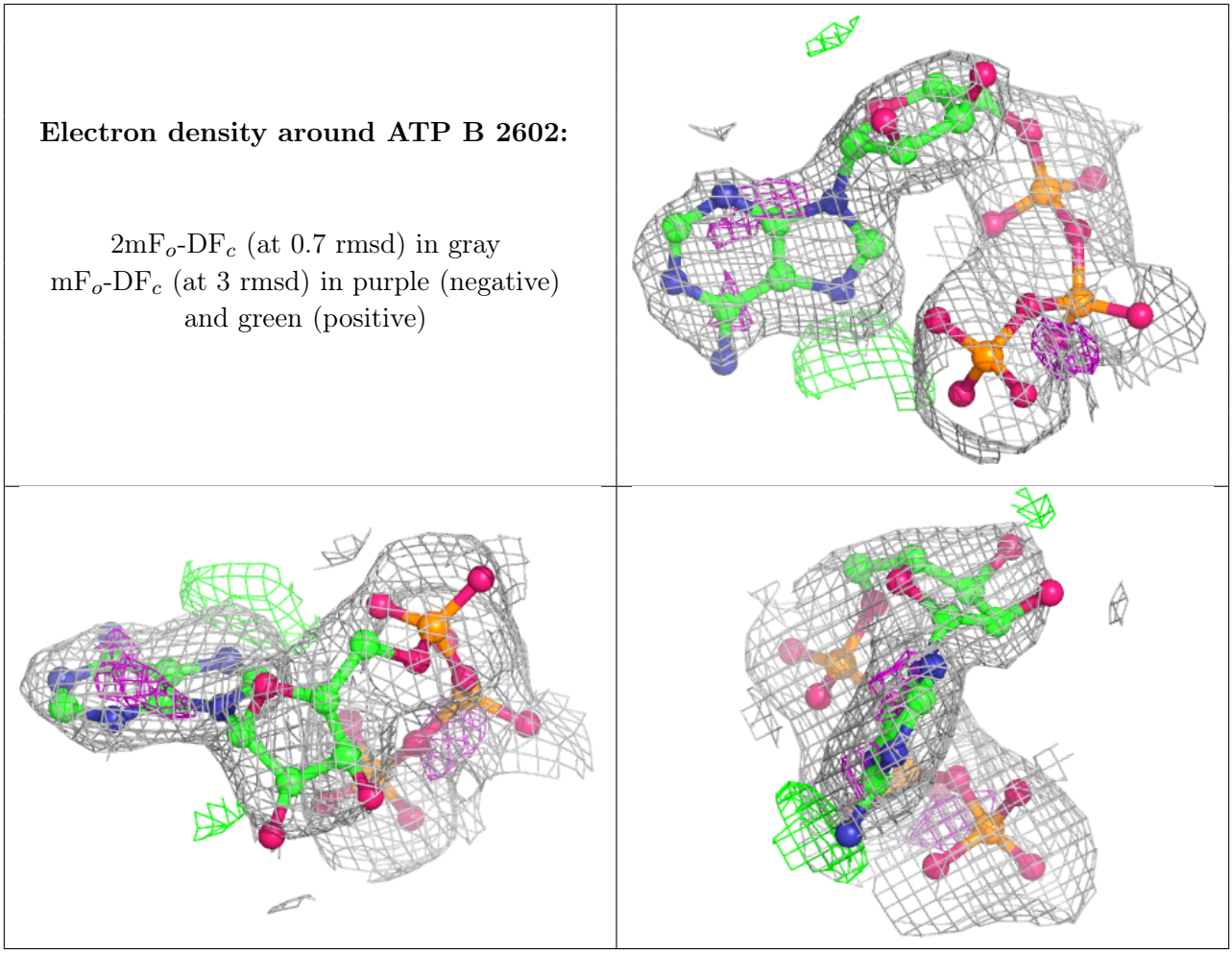
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





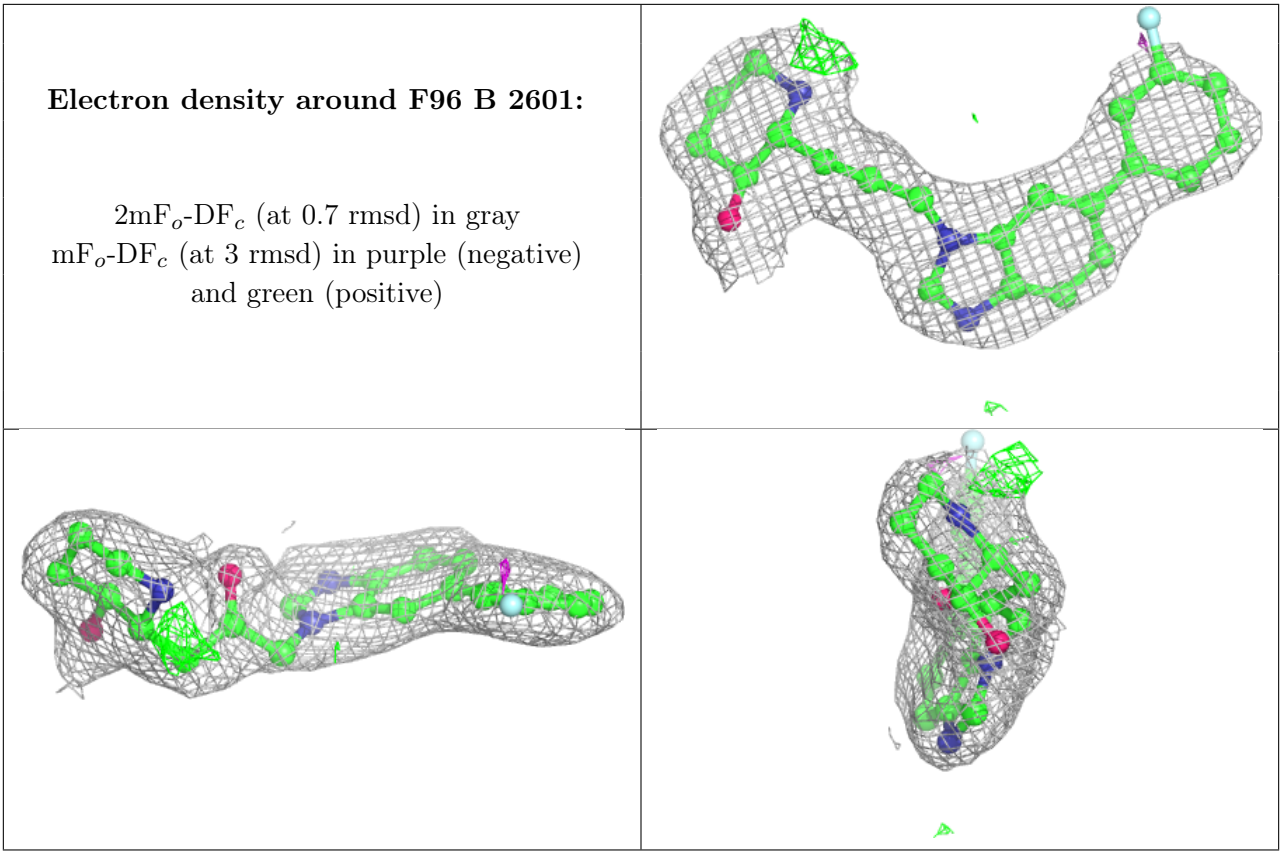
Electron density around ATP B 2602:

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



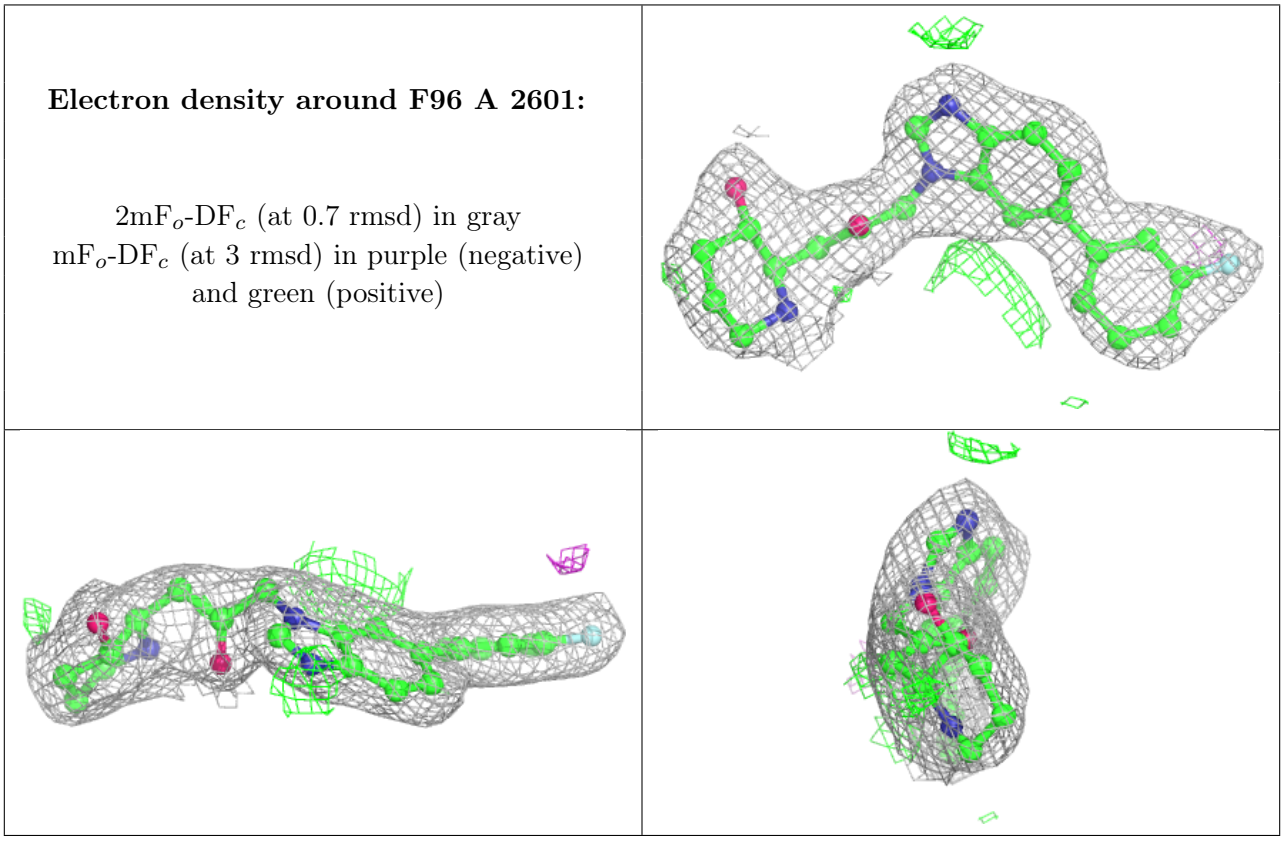
Electron density around F96 B 2601:

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



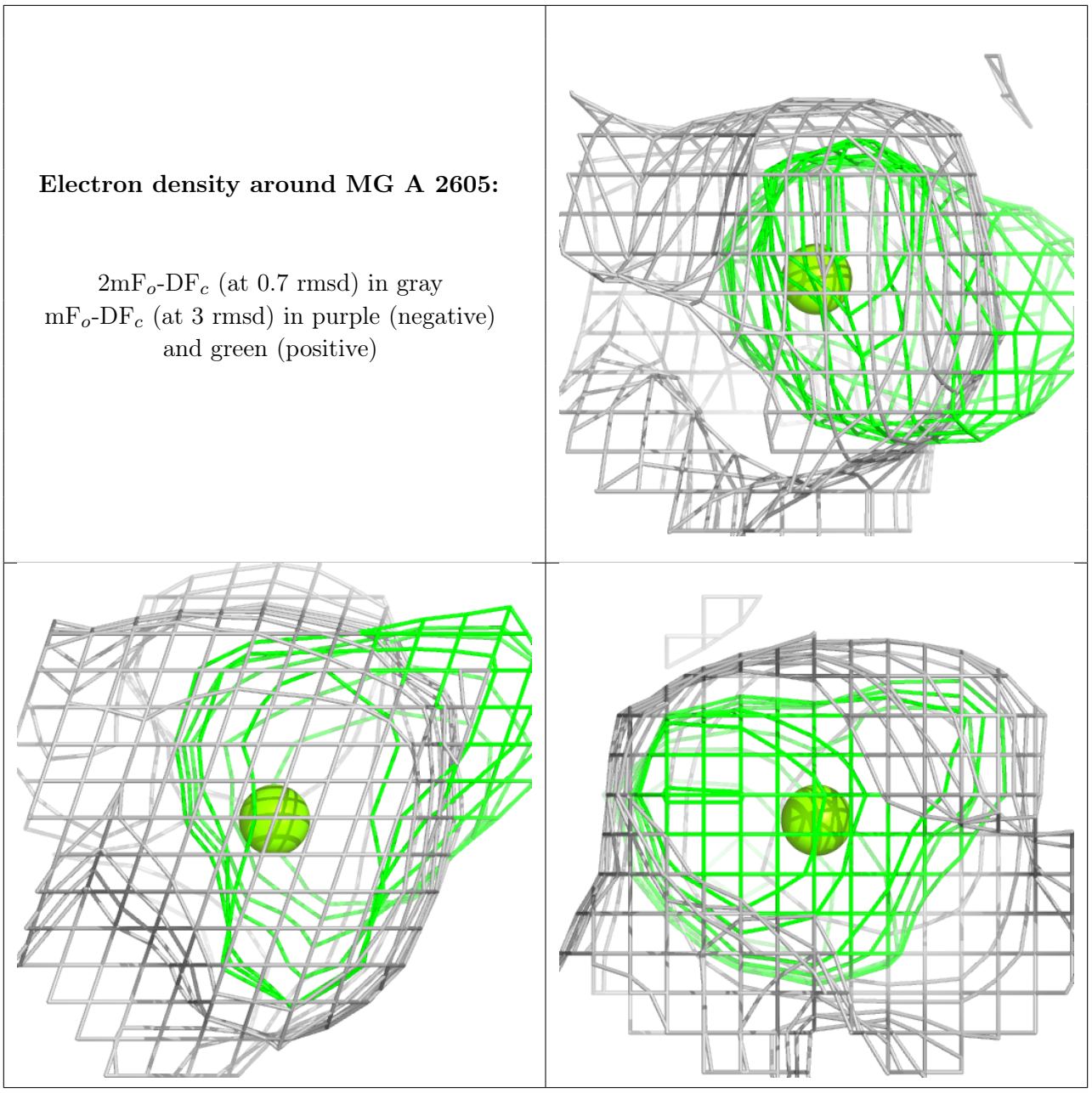
Electron density around F96 A 2601:

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



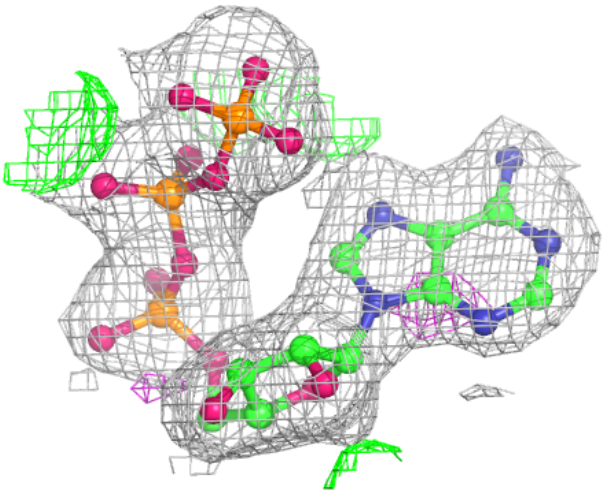
Electron density around MG A 2605:

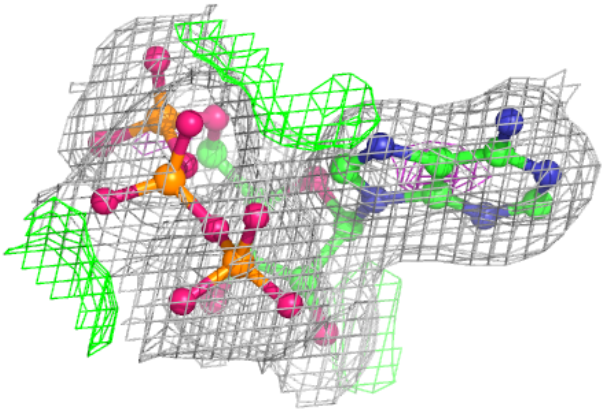
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

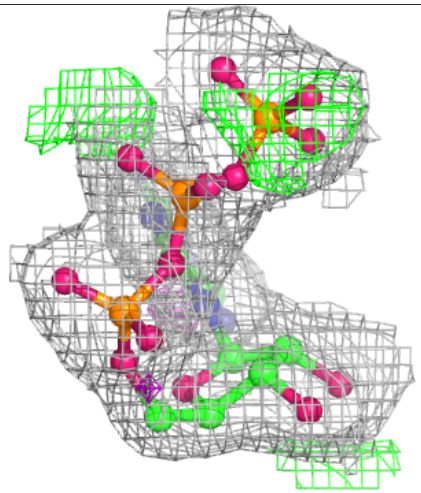


Electron density around ATP A 2602:

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

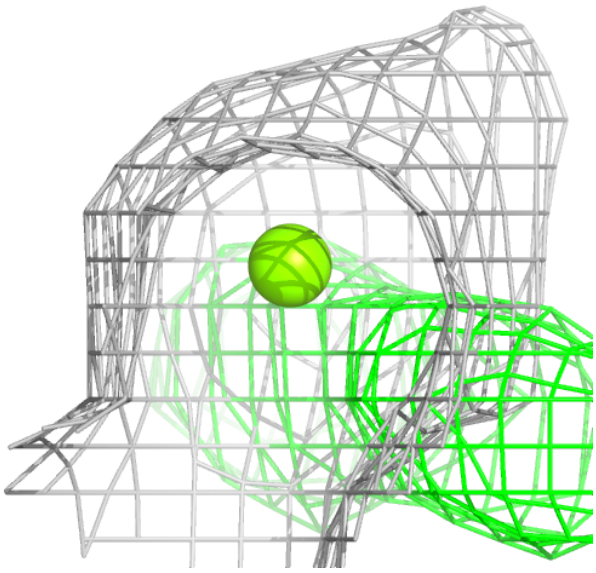


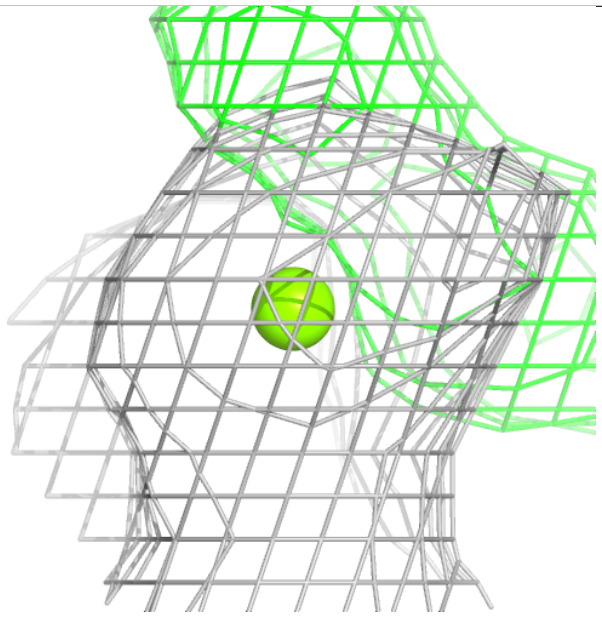


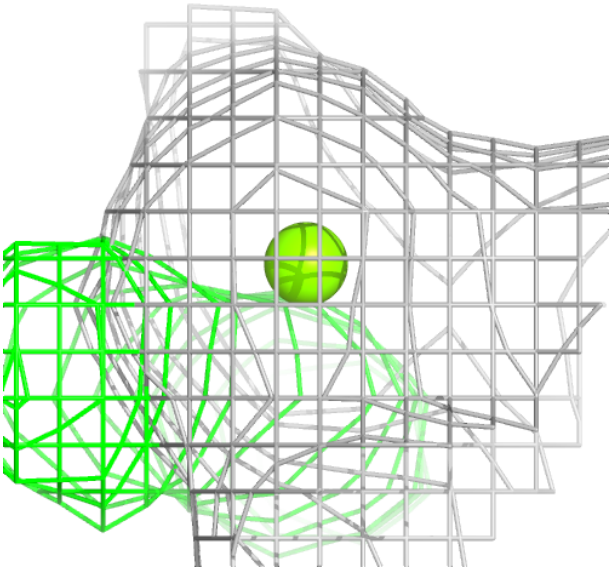


Electron density around MG A 2604:

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

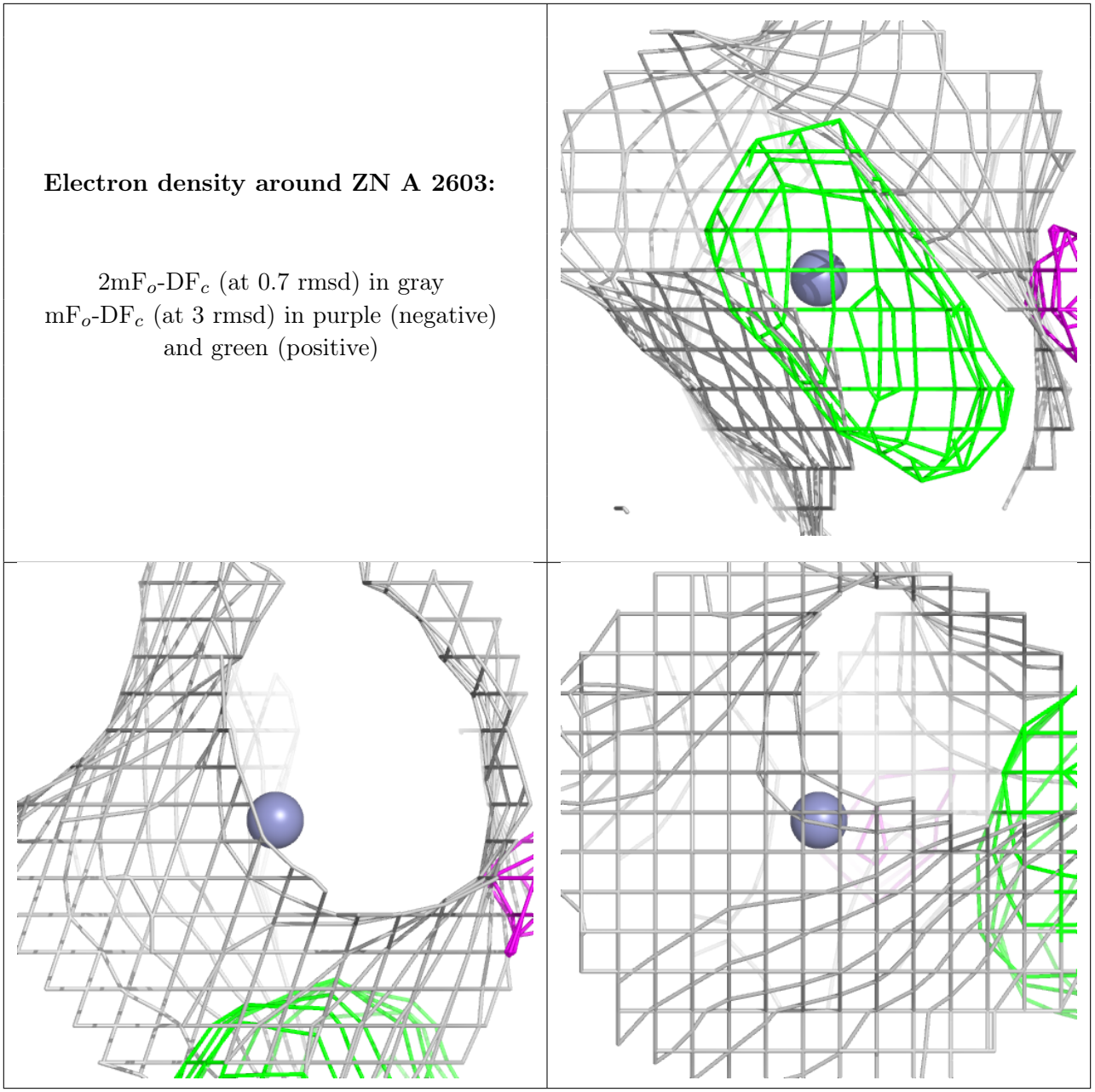






Electron density around ZN A 2603:

$2mF_o$-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.