Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2026 – 05:47 am BST

PDB ID	:	7OAR / pdb_00007oar
Title	:	Crystal structure of helicase Pif1 from Thermus oshimai in complex with parallel G-quadruplex
Authors	:	Dai, Y.X.; Liu, N.N.; Guo, H.L.; Chen, W.F.; Rety, S.; Xi, X.G.
Deposited on	:	2021-04-20
Resolution	:	2.58 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:

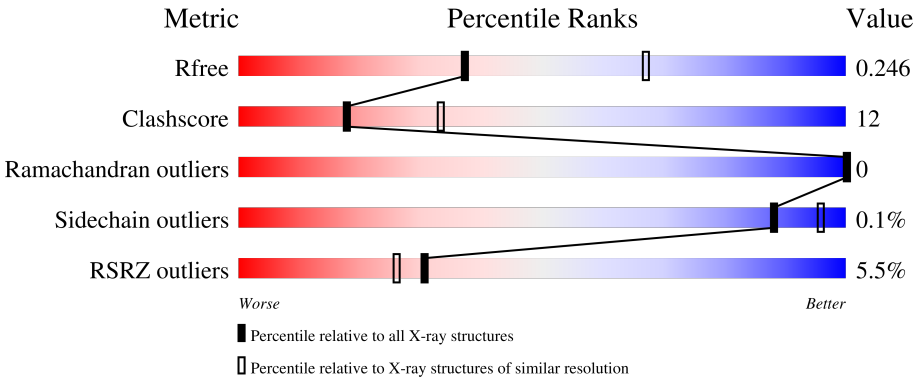
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	450	3% 76% 22% ·
1	B	450	8% 69% 22% · 8%
2	C	29	83% 14% ·

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7528 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.

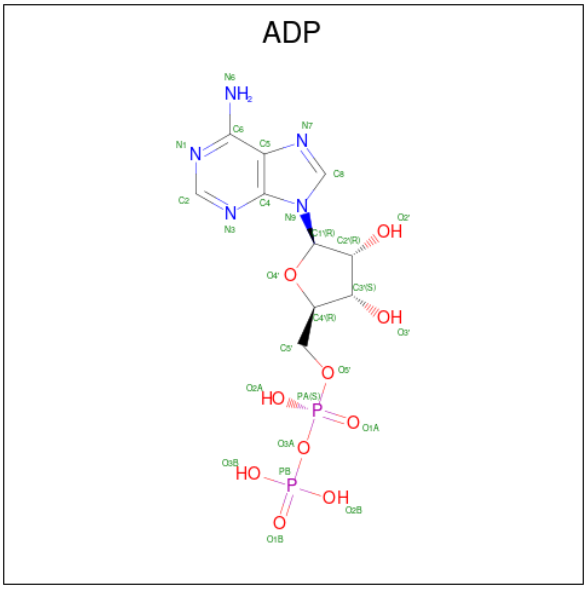
- Molecule 1 is a protein called Pif1 helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3552	2274	648	627	3			
1	B	413	Total	C	N	O	S	0	0	0
			3304	2111	609	581	3			

- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	28	Total	C	N	O	P	0	0	0
			565	270	90	178	27			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued on next page...

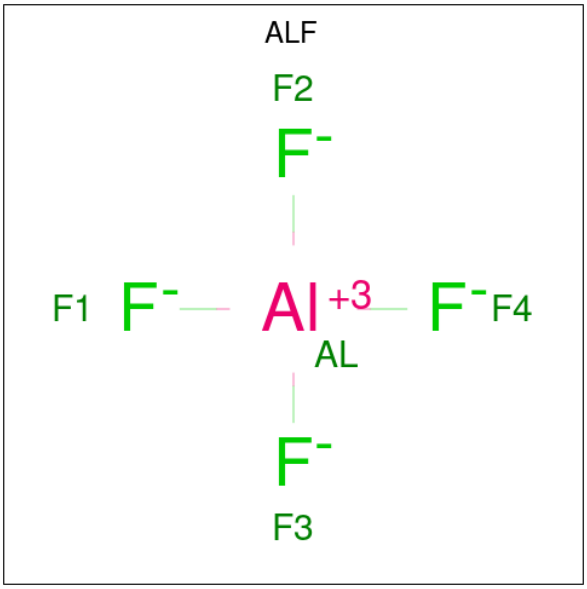
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			5	1	4		
5	B	1	Total	Al	F	0	0
			5	1	4		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	3	Total K 3 3	0	0

- Molecule 7 is water.

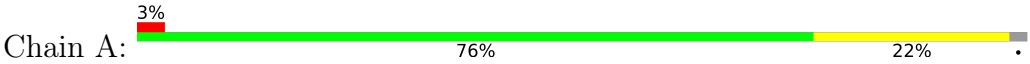
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	17	Total O 17 17	0	0
7	B	21	Total O 21 21	0	0

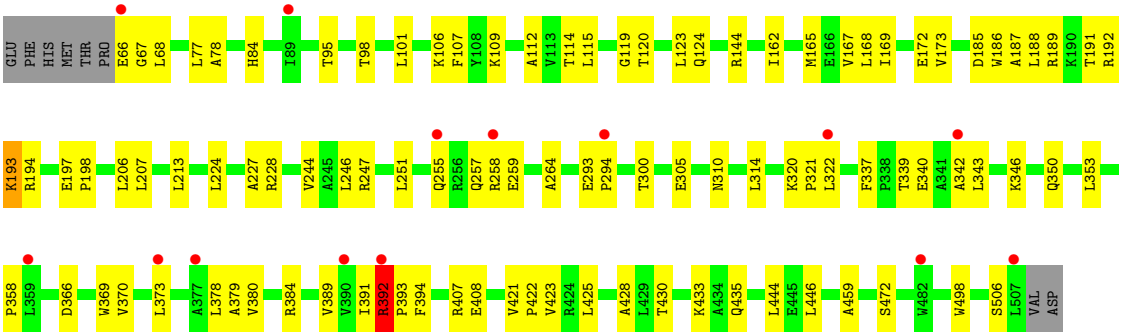
3 Residue-property plots (i)

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: Pif1 helicase

Chain A:

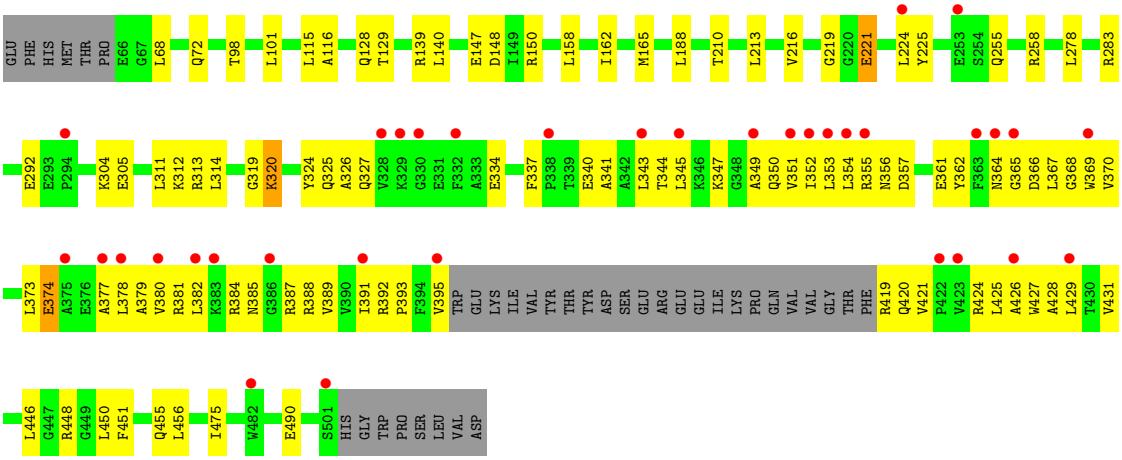




• Molecule 1: Pif1 helicase

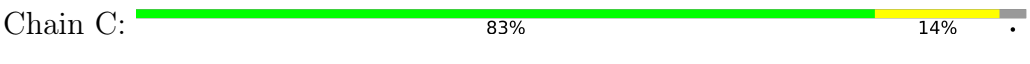
Chain B:

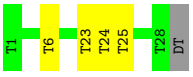




• Molecule 2: DNA (28-MER)

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	151.78Å 151.78Å 219.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.39 – 2.58 37.39 – 2.58	Depositor EDS
% Data completeness (in resolution range)	93.6 (37.39-2.58) 93.6 (37.39-2.58)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.58Å)	Xtriage
Refinement program	PHENIX dev_3512, PHENIX dev_3512	Depositor
R, R_{free}	0.194 , 0.243 0.202 , 0.246	Depositor DCC
R_{free} test set	2130 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å^2)	87.6	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 83.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7528	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: K, ADP, ALF, 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	0.42	1/3638 (0.0%)	0.66	5/4938 (0.1%)
1	B	0.38	0/3379	0.63	0/4582
2	C	0.35	0/630	0.57	0/977
All	All	0.39	1/7647 (0.0%)	0.64	5/10497 (0.0%)

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	4
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	ARG	C-N	13.61	1.50	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	392	ARG	CA-C-N	14.70	134.89	119.90
1	A	392	ARG	C-N-CA	14.70	134.89	119.90
1	A	193	LYS	CA-CB-CG	5.65	125.40	114.10
1	A	66	GLU	CA-C-N	-5.34	110.94	121.41
1	A	66	GLU	C-N-CA	-5.34	110.94	121.41

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	GLY	Peptide
1	B	219	GLY	Peptide
1	B	221	GLU	Peptide
1	B	320	LYS	Peptide
1	B	374	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	3552	0	3610	81	0
1	B	3304	0	3376	99	0
2	C	565	0	313	4	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	C	3	0	0	0	0
7	A	17	0	0	2	0
7	B	21	0	0	2	0
All	All	7528	0	7323	181	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 (181) 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:106:LYS:O	1:A:109:LYS:HE3	1.66	0.94
1:B:382:LEU:HD11	1:B:389:VAL:HG13	1.52	0.90
1:B:326:ALA:HB2	1:B:420:GLN:HB2	1.56	0.87
1:B:324:TYR:HB3	1:B:420:GLN:NE2	1.93	0.84
1:B:357:ASP:HB3	1:B:362:TYR:CZ	2.20	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HD12	1:A:366:ASP:HB3	1.67	0.77
1:B:370:VAL:HG23	1:B:380:VAL:HG12	1.66	0.75
1:B:431:VAL:HG21	1:B:455:GLN:HG3	1.68	0.75
1:B:393:PRO:HD3	1:B:421:VAL:HG12	1.67	0.74
1:B:347:LYS:HA	1:B:370:VAL:CG1	2.18	0.74
1:A:106:LYS:O	1:A:109:LYS:CE	2.35	0.73
1:B:385:ASN:HB3	1:B:387:ARG:HB2	1.68	0.73
1:B:347:LYS:HA	1:B:370:VAL:HG13	1.73	0.70
1:B:352:ILE:HB	1:B:367:LEU:HB3	1.73	0.70
1:A:106:LYS:CE	1:A:109:LYS:HG3	2.23	0.69
1:B:366:ASP:OD2	1:B:384:ARG:HB3	1.93	0.69
1:A:106:LYS:NZ	1:A:109:LYS:HG3	2.08	0.67
1:A:407:ARG:HH11	1:A:407:ARG:HB3	1.58	0.67
1:A:370:VAL:HG23	1:A:378:LEU:HD21	1.76	0.67
1:A:392:ARG:C	1:A:392:ARG:HD2	2.20	0.67
1:A:366:ASP:OD2	1:A:384:ARG:NH1	2.28	0.67
1:B:139:ARG:NH1	1:B:148:ASP:OD1	2.29	0.66
1:A:407:ARG:HB3	1:A:407:ARG:NH1	2.12	0.65
1:A:393:PRO:HG3	1:A:421:VAL:HG12	1.78	0.65
1:A:389:VAL:HG23	1:A:391:ILE:HD11	1.78	0.65
1:B:392:ARG:HG2	1:B:393:PRO:HD2	1.80	0.64
1:A:392:ARG:HH11	1:A:392:ARG:HG3	1.62	0.63
1:B:420:GLN:NE2	1:B:421:VAL:HG22	2.13	0.63
1:A:300:THR:HG21	1:A:305:GLU:HB2	1.79	0.63
1:B:162:ILE:HA	1:B:165:MET:HE3	1.81	0.63
1:B:324:TYR:HB3	1:B:420:GLN:HE21	1.63	0.62
1:B:352:ILE:HG22	1:B:426:ALA:HB2	1.81	0.62
1:B:312:LYS:NZ	1:B:312:LYS:HB3	2.14	0.62
1:A:106:LYS:HA	1:A:106:LYS:HE2	1.80	0.62
1:B:395:VAL:HG12	1:B:419:ARG:HB2	1.82	0.61
1:A:369:TRP:C	1:A:380:VAL:HG23	2.26	0.61
1:B:221:GLU:HB3	1:B:224:LEU:HD23	1.83	0.61
1:B:362:TYR:HB3	1:B:389:VAL:HG11	1.83	0.60
1:B:370:VAL:HA	1:B:380:VAL:HA	1.83	0.59
1:B:451:PHE:CZ	2:C:23:DT:H2"	2.37	0.59
1:A:144:ARG:HG2	1:A:186:TRP:CG	2.38	0.58
1:B:319:GLY:O	1:B:320:LYS:HD3	2.04	0.58
1:B:350:GLN:HA	1:B:368:GLY:O	2.03	0.57
1:A:112:ALA:HA	1:A:167:VAL:O	2.03	0.57
1:B:450:LEU:HD13	1:B:456:LEU:HB2	1.86	0.57
1:A:68:LEU:H	1:A:68:LEU:HD22	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:GLU:HA	1:A:408:GLU:OE1	2.05	0.56
1:A:188:LEU:O	1:A:192:ARG:HB2	2.05	0.56
1:A:380:VAL:HG12	1:A:391:ILE:CD1	2.36	0.56
1:B:334:GLU:HA	1:B:337:PHE:HE2	1.69	0.56
1:B:448:ARG:HD3	7:B:1108:HOH:O	2.03	0.56
1:A:106:LYS:HE2	1:A:109:LYS:HG3	1.88	0.56
1:A:119:GLY:O	1:A:123:LEU:HG	2.05	0.56
1:B:428:ALA:O	1:B:429:LEU:HD23	2.05	0.56
1:A:421:VAL:HG23	1:A:423:VAL:HG12	1.87	0.55
1:A:162:ILE:HA	1:A:165:MET:HE3	1.88	0.55
1:A:192:ARG:O	1:A:193:LYS:HB3	2.05	0.55
1:A:258:ARG:HG3	1:A:259:GLU:HG3	1.88	0.55
1:B:221:GLU:HB3	1:B:224:LEU:CD2	2.36	0.55
1:B:340:GLU:H	1:B:340:GLU:CD	2.15	0.55
1:B:352:ILE:HD11	1:B:365:GLY:C	2.31	0.55
1:B:420:GLN:HE21	1:B:421:VAL:HG22	1.71	0.55
1:A:391:ILE:HD12	1:A:391:ILE:N	2.22	0.55
1:A:300:THR:CG2	1:A:305:GLU:HB2	2.36	0.54
1:A:369:TRP:O	1:A:380:VAL:HG23	2.08	0.54
1:B:393:PRO:HD3	1:B:421:VAL:CG1	2.34	0.54
1:B:392:ARG:C	1:B:392:ARG:HD3	2.33	0.54
1:A:358:PRO:HD3	1:A:394:PHE:HZ	1.74	0.53
1:B:373:LEU:CD1	1:B:378:LEU:HD23	2.38	0.53
1:A:172:GLU:OE1	1:A:435:GLN:HG2	2.09	0.53
1:A:193:LYS:O	1:A:193:LYS:HG2	2.09	0.53
1:A:194:ARG:NH2	1:A:197:GLU:HG3	2.24	0.52
1:B:379:ALA:HB1	1:B:388:ARG:NH2	2.24	0.52
1:B:147:GLU:HG2	1:B:150:ARG:NH2	2.25	0.52
1:B:216:VAL:HG21	2:C:25:DT:C2	2.44	0.52
1:A:84:HIS:CD2	1:A:247:ARG:HG3	2.44	0.52
1:A:106:LYS:CE	1:A:106:LYS:HA	2.40	0.52
1:B:325:GLN:HG2	1:B:326:ALA:H	1.75	0.52
1:B:420:GLN:HA	1:B:420:GLN:OE1	2.10	0.52
1:A:162:ILE:HG22	1:A:192:ARG:HG3	1.92	0.51
1:B:278:LEU:HD11	1:B:475:ILE:HB	1.93	0.51
1:B:392:ARG:HD3	1:B:393:PRO:O	2.11	0.50
1:B:68:LEU:HD22	1:B:72:GLN:HB3	1.93	0.50
1:A:98:THR:O	1:A:101:LEU:HB3	2.11	0.50
1:B:334:GLU:HA	1:B:337:PHE:CE2	2.46	0.50
1:A:124:GLN:HG2	7:A:1111:HOH:O	2.12	0.49
1:A:173:VAL:HG21	1:A:206:LEU:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ALA:O	1:A:191:THR:HG23	2.12	0.49
1:A:380:VAL:HG12	1:A:391:ILE:HD13	1.94	0.49
1:B:311:LEU:HD12	1:B:312:LYS:N	2.27	0.49
1:B:361:GLU:OE1	1:B:387:ARG:NH1	2.45	0.49
1:B:340:GLU:OE1	1:B:340:GLU:N	2.40	0.48
1:B:379:ALA:CB	1:B:388:ARG:HH22	2.26	0.48
1:B:140:LEU:HD21	1:B:225:TYR:CD1	2.49	0.48
1:B:374:GLU:OE2	1:B:377:ALA:HB3	2.14	0.48
1:B:379:ALA:HB1	1:B:388:ARG:HH22	1.79	0.48
1:A:109:LYS:O	1:A:109:LYS:HG2	2.13	0.48
1:A:392:ARG:HG3	1:A:392:ARG:NH1	2.28	0.48
1:B:351:VAL:HB	1:B:424:ARG:O	2.14	0.48
1:A:172:GLU:OE2	7:A:1101:HOH:O	2.20	0.47
2:C:24:DT:H72	2:C:25:DT:H73	1.96	0.47
1:A:255:GLN:O	1:A:258:ARG:HD2	2.14	0.47
1:A:198:PRO:HG2	1:A:244:VAL:HB	1.96	0.47
1:B:351:VAL:CG1	1:B:425:LEU:HD23	2.44	0.47
1:B:373:LEU:HD11	1:B:378:LEU:HD23	1.95	0.47
1:A:337:PHE:HB3	1:A:339:THR:O	2.15	0.46
1:B:378:LEU:HB2	1:B:391:ILE:O	2.15	0.46
1:B:351:VAL:HB	1:B:425:LEU:HA	1.97	0.46
1:A:107:PHE:CD1	1:A:107:PHE:C	2.93	0.46
1:A:322:LEU:HD23	1:A:373:LEU:HG	1.98	0.46
1:B:343:LEU:HD12	1:B:343:LEU:HA	1.53	0.46
1:B:349:ALA:HB1	1:B:427:TRP:CH2	2.51	0.46
1:B:352:ILE:HD12	1:B:367:LEU:HD22	1.98	0.46
1:B:352:ILE:HG13	1:B:366:ASP:C	2.41	0.46
1:B:384:ARG:NH1	1:B:385:ASN:HB2	2.31	0.46
1:A:378:LEU:HD22	1:A:379:ALA:H	1.81	0.46
1:B:388:ARG:NH1	1:B:389:VAL:O	2.49	0.46
1:A:393:PRO:HA	1:A:421:VAL:HA	1.98	0.45
1:B:392:ARG:HD3	1:B:393:PRO:N	2.31	0.45
1:B:340:GLU:HG2	1:B:343:LEU:HD13	1.98	0.45
1:A:115:LEU:HD12	1:A:168:LEU:HD11	1.98	0.45
1:B:353:LEU:HD13	1:B:366:ASP:O	2.17	0.45
1:B:431:VAL:HG22	7:B:1118:HOH:O	2.17	0.45
1:A:106:LYS:HZ3	1:A:109:LYS:HG3	1.80	0.45
1:B:354:LEU:HD11	1:B:424:ARG:HB2	1.99	0.45
1:B:325:GLN:HG3	1:B:341:ALA:O	2.17	0.44
1:A:293:GLU:HG3	1:A:294:PRO:HD2	1.99	0.44
1:A:300:THR:O	1:A:430:THR:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LYS:HG3	1:A:321:PRO:HD2	1.99	0.44
1:B:446:LEU:HD11	1:B:475:ILE:HD11	1.99	0.44
1:A:114:THR:HA	1:A:169:ILE:O	2.18	0.44
1:B:213:LEU:HD11	1:B:431:VAL:HG23	2.00	0.44
1:B:158:LEU:O	1:B:162:ILE:HG13	2.17	0.43
1:A:380:VAL:HG12	1:A:391:ILE:HD11	1.99	0.43
1:B:115:LEU:HA	1:B:128:GLN:O	2.19	0.43
1:B:283:ARG:CZ	1:B:283:ARG:HB2	2.47	0.43
1:A:213:LEU:HB2	1:A:435:GLN:OE1	2.18	0.43
1:A:339:THR:OG1	1:A:343:LEU:HD12	2.19	0.43
1:B:304:LYS:HD2	1:B:304:LYS:C	2.43	0.43
1:A:95:THR:HG21	1:A:251:LEU:C	2.43	0.42
1:B:116:ALA:O	1:B:129:THR:HA	2.18	0.42
1:A:340:GLU:HG3	1:A:342:ALA:H	1.84	0.42
1:B:384:ARG:NH1	1:B:385:ASN:HD22	2.17	0.42
1:A:310:ASN:OD1	1:A:428:ALA:N	2.52	0.42
1:B:393:PRO:HB3	1:B:420:GLN:C	2.44	0.42
1:A:109:LYS:HE3	1:A:109:LYS:HB2	1.70	0.42
1:A:257:GLN:HB2	1:A:264:ALA:HB2	2.02	0.42
1:B:344:THR:O	1:B:345:LEU:HD23	2.20	0.42
1:B:351:VAL:HG12	1:B:425:LEU:HD23	2.02	0.42
1:B:366:ASP:OD2	1:B:382:LEU:HB3	2.20	0.42
1:A:120:THR:HG21	1:A:433:LYS:O	2.20	0.42
1:A:246:LEU:HB3	1:A:498:TRP:HB3	2.02	0.42
1:B:369:TRP:O	1:B:381:ARG:N	2.47	0.42
1:B:314:LEU:HD21	1:B:344:THR:OG1	2.20	0.42
1:B:325:GLN:HG2	1:B:326:ALA:N	2.34	0.42
1:B:283:ARG:HB2	1:B:283:ARG:NH1	2.35	0.41
1:B:292:GLU:HA	1:B:313:ARG:HH12	1.85	0.41
1:B:255:GLN:O	1:B:258:ARG:HD2	2.20	0.41
1:A:310:ASN:ND2	1:A:425:LEU:O	2.53	0.41
1:A:77:LEU:HD12	1:A:78:ALA:N	2.35	0.41
1:A:227:ALA:O	1:A:506:SER:HB2	2.21	0.41
1:A:350:GLN:HG2	1:A:369:TRP:NE1	2.35	0.41
1:B:356:ASN:OD1	1:B:364:ASN:N	2.43	0.41
1:B:395:VAL:CG1	1:B:419:ARG:HB2	2.49	0.41
1:A:185:ASP:CG	1:A:189:ARG:HE	2.28	0.41
1:B:162:ILE:HG23	1:B:188:LEU:HD23	2.02	0.41
1:A:224:LEU:O	1:A:228:ARG:HG3	2.20	0.41
1:B:304:LYS:HD2	1:B:305:GLU:N	2.34	0.41
1:B:370:VAL:CG2	1:B:380:VAL:HG12	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD12	1:A:207:LEU:HD13	2.03	0.41
1:B:351:VAL:CG1	1:B:425:LEU:HA	2.51	0.41
1:B:428:ALA:C	1:B:429:LEU:HD23	2.46	0.41
1:B:210:THR:OG1	1:B:490:GLU:OE2	2.39	0.41
1:A:314:LEU:HD11	1:A:346:LYS:H	1.86	0.40
1:B:98:THR:O	1:B:101:LEU:HB3	2.21	0.40
1:B:327:GLN:HG2	1:B:419:ARG:HD2	2.04	0.40
1:A:392:ARG:NH2	2:C:6:DT:O4	2.55	0.40
1:A:444:LEU:HD13	1:A:459:ALA:HB1	2.03	0.40
1:A:446:LEU:HD23	1:A:472:SER:HB3	2.04	0.40
1:A:394:PHE:CD1	1:A:422:PRO:HG3	2.57	0.40
1:B:354:LEU:O	1:B:355:ARG:HG2	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	440/450 (98%)	439 (100%)	1 (0%)	0	100	100
1	B	409/450 (91%)	408 (100%)	1 (0%)	0	100	100
All	All	849/900 (94%)	847 (100%)	2 (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	369/377 (98%)	368 (100%)	1 (0%)	86 94
1	B	342/377 (91%)	342 (100%)	0	100 100
All	All	711/754 (94%)	710 (100%)	1 (0%)	88 96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	GLN
1	A	453	HIS
1	B	145	HIS
1	B	364	ASN
1	B	385	ASN
1	B	420	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 5 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	$\#\|Z\| > 2$
3	ADP	B	1001	5,4	27,29,29	1.59	4 (14%)	42,45,45	1.82	11 (26%)
3	ADP	A	1001	5,4	27,29,29	1.39	4 (14%)	42,45,45	1.85	12 (28%)
5	ALF	B	1003	3,7	0,4,4	-	-	-		
5	ALF	A	1003	3,7	0,4,4	-	-	-		

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	ADP	B	1001	5,4	-	2/16/32/32	0/3/3/3
3	ADP	A	1001	5,4	-	4/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	ADP	C5-C4	4.74	1.47	1.39
3	A	1001	ADP	C5-C4	4.61	1.47	1.39
3	B	1001	ADP	C5-C6	2.98	1.49	1.41
3	B	1001	ADP	PB-O3B	-2.88	1.43	1.54
3	B	1001	ADP	C8-N7	2.65	1.36	1.31
3	A	1001	ADP	C8-N7	2.65	1.36	1.31
3	A	1001	ADP	C5-C6	2.57	1.48	1.41
3	A	1001	ADP	C4-N9	-2.35	1.32	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1001	ADP	C5-C4-N3	-5.50	119.58	126.75
3	A	1001	ADP	C5-C4-N3	-4.88	120.39	126.75
3	B	1001	ADP	C4-C5-N7	-4.14	105.58	110.62
3	A	1001	ADP	N3-C4-N9	4.03	133.72	127.08
3	B	1001	ADP	N3-C4-N9	3.71	133.20	127.08
3	A	1001	ADP	C4-N9-C8	3.51	109.53	105.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	ADP	N3-C2-N1	-3.36	123.35	128.60
3	A	1001	ADP	C2-N3-C4	3.34	119.65	111.75
3	B	1001	ADP	C2-N3-C4	3.30	119.55	111.75
3	A	1001	ADP	C4-C5-N7	-3.05	106.90	110.62
3	B	1001	ADP	C5-N7-C8	3.02	107.81	103.51
3	B	1001	ADP	C6-C5-N7	2.82	137.28	132.02
3	B	1001	ADP	O3'-C3'-C4'	-2.76	103.07	111.05
3	A	1001	ADP	C2-N1-C6	2.54	123.13	118.77
3	B	1001	ADP	N3-C2-N1	-2.52	124.65	128.60
3	B	1001	ADP	C4-N9-C8	2.36	108.28	105.73
3	A	1001	ADP	C6-C5-N7	2.36	136.41	132.02
3	A	1001	ADP	C5-N7-C8	2.34	106.83	103.51
3	A	1001	ADP	O2A-PA-O1A	2.27	123.47	112.24
3	A	1001	ADP	O3A-PB-O1B	-2.27	98.59	111.19
3	A	1001	ADP	N9-C8-N7	-2.24	110.85	113.91
3	B	1001	ADP	N9-C8-N7	-2.05	111.11	113.91
3	B	1001	ADP	C2-N1-C6	2.02	122.23	118.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	ADP	C5'-O5'-PA-O2A
3	B	1001	ADP	PA-O3A-PB-O2B
3	A	1001	ADP	C5'-O5'-PA-O3A
3	A	1001	ADP	C5'-O5'-PA-O1A
3	A	1001	ADP	O4'-C4'-C5'-O5'
3	B	1001	ADP	PA-O3A-PB-O1B

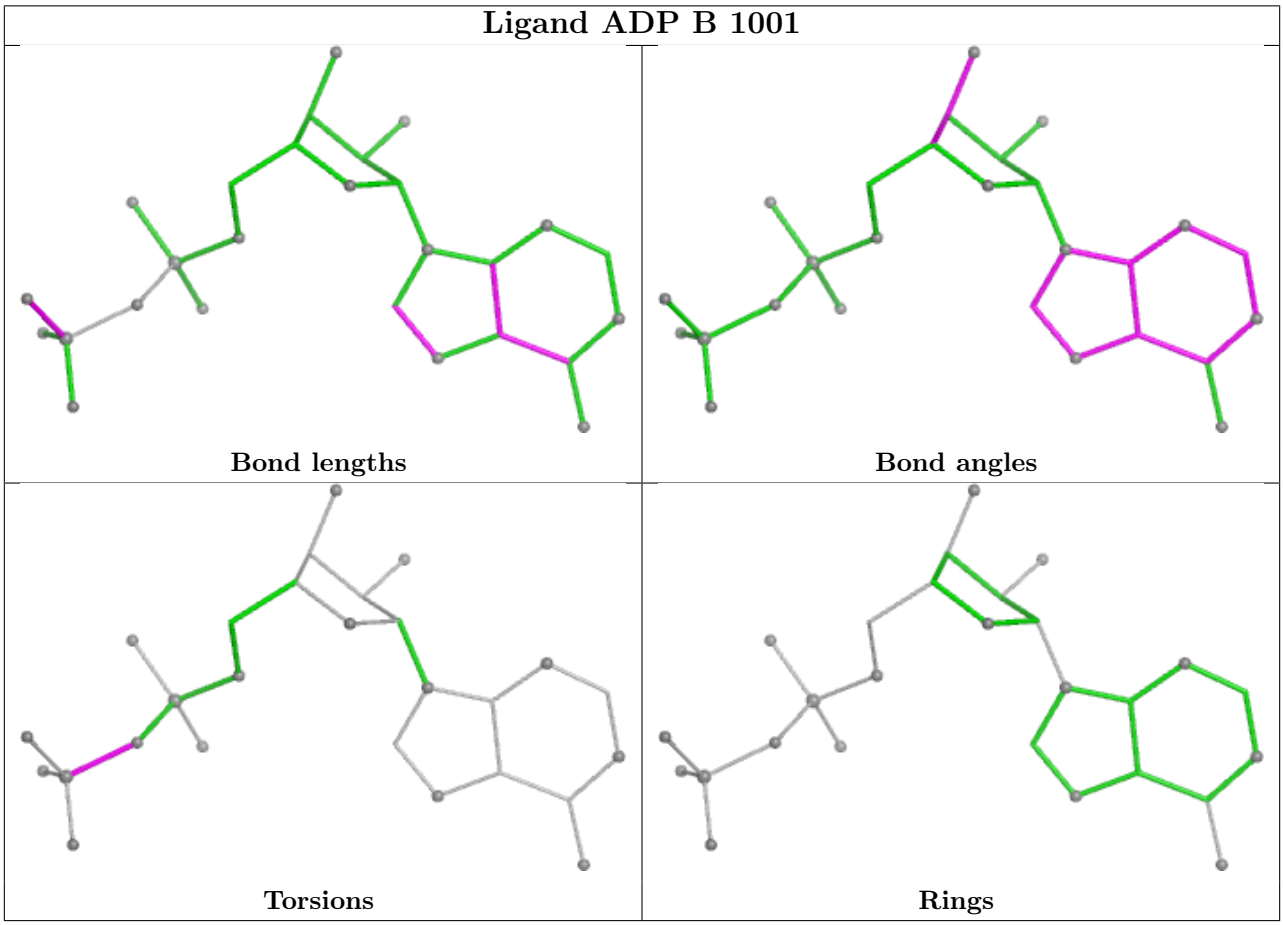
There are no ring outliers.

No monomer is involved in short contacts.

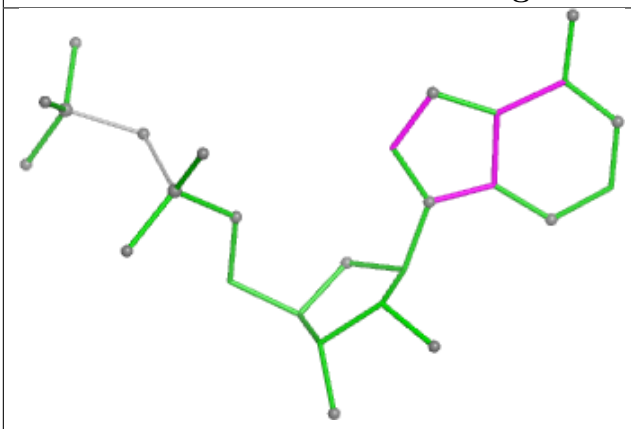
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

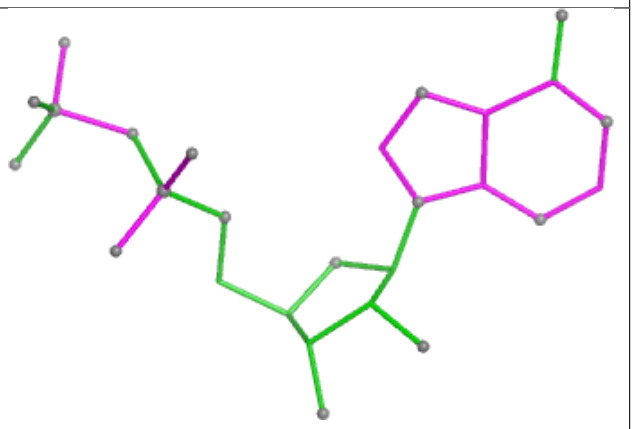
Ligand ADP B 1001



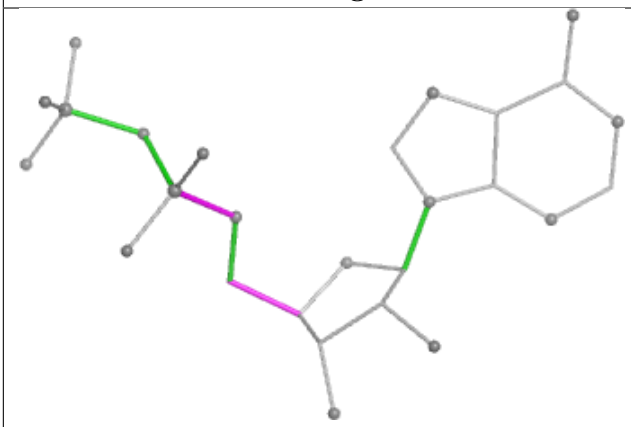
Ligand ADP A 1001



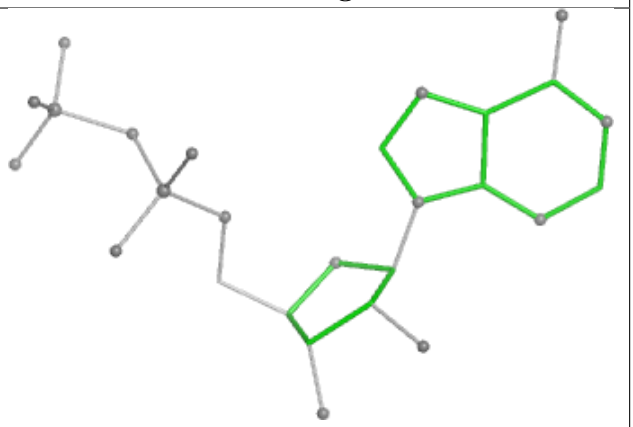
Bond lengths



Bond angles

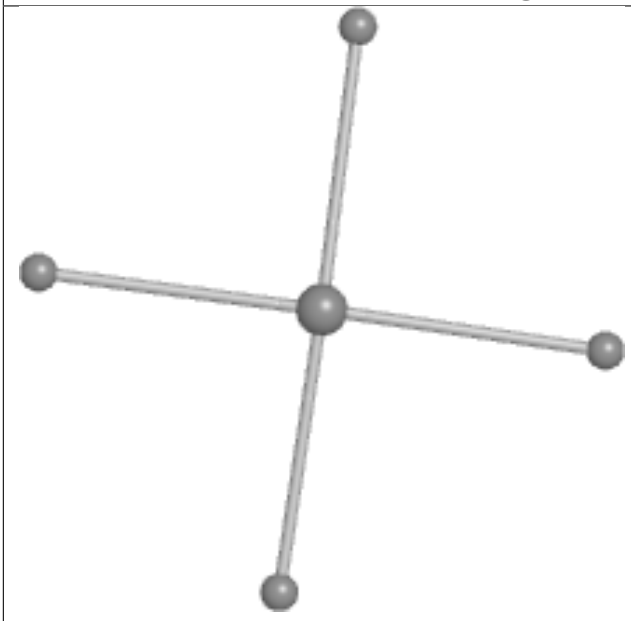


Torsions

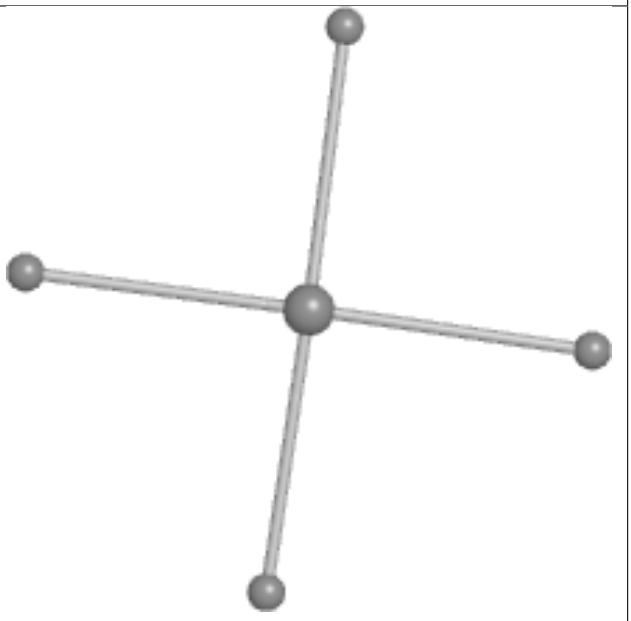


Rings

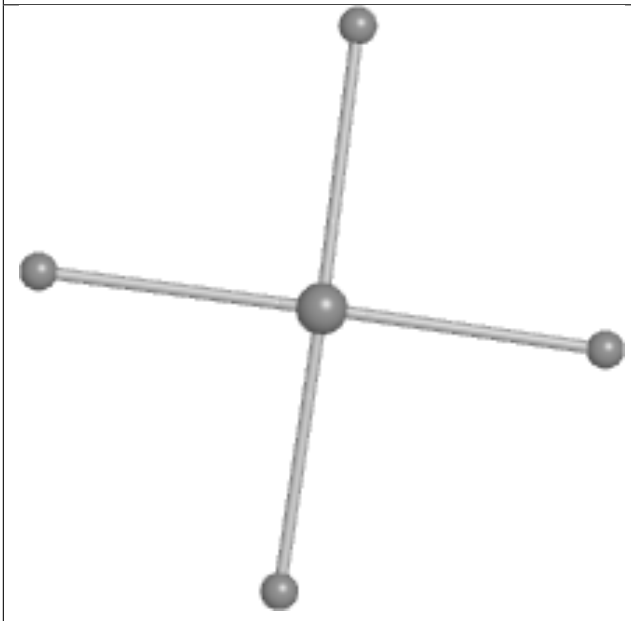
Ligand ALF B 1003



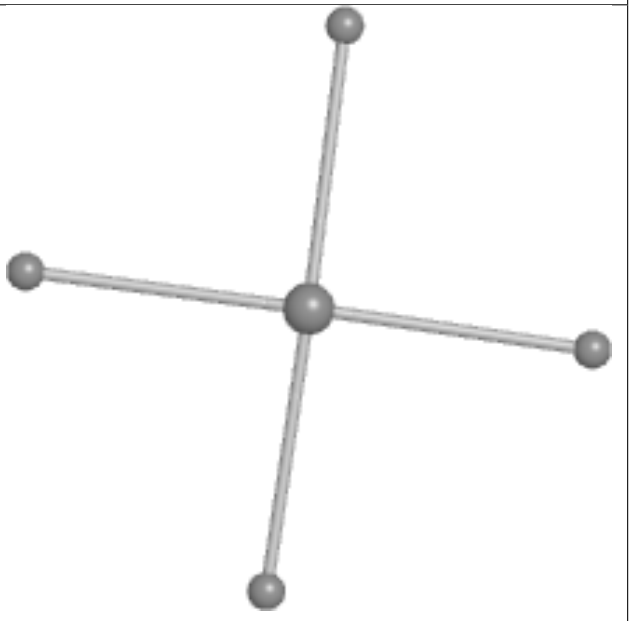
Bond lengths



Bond angles

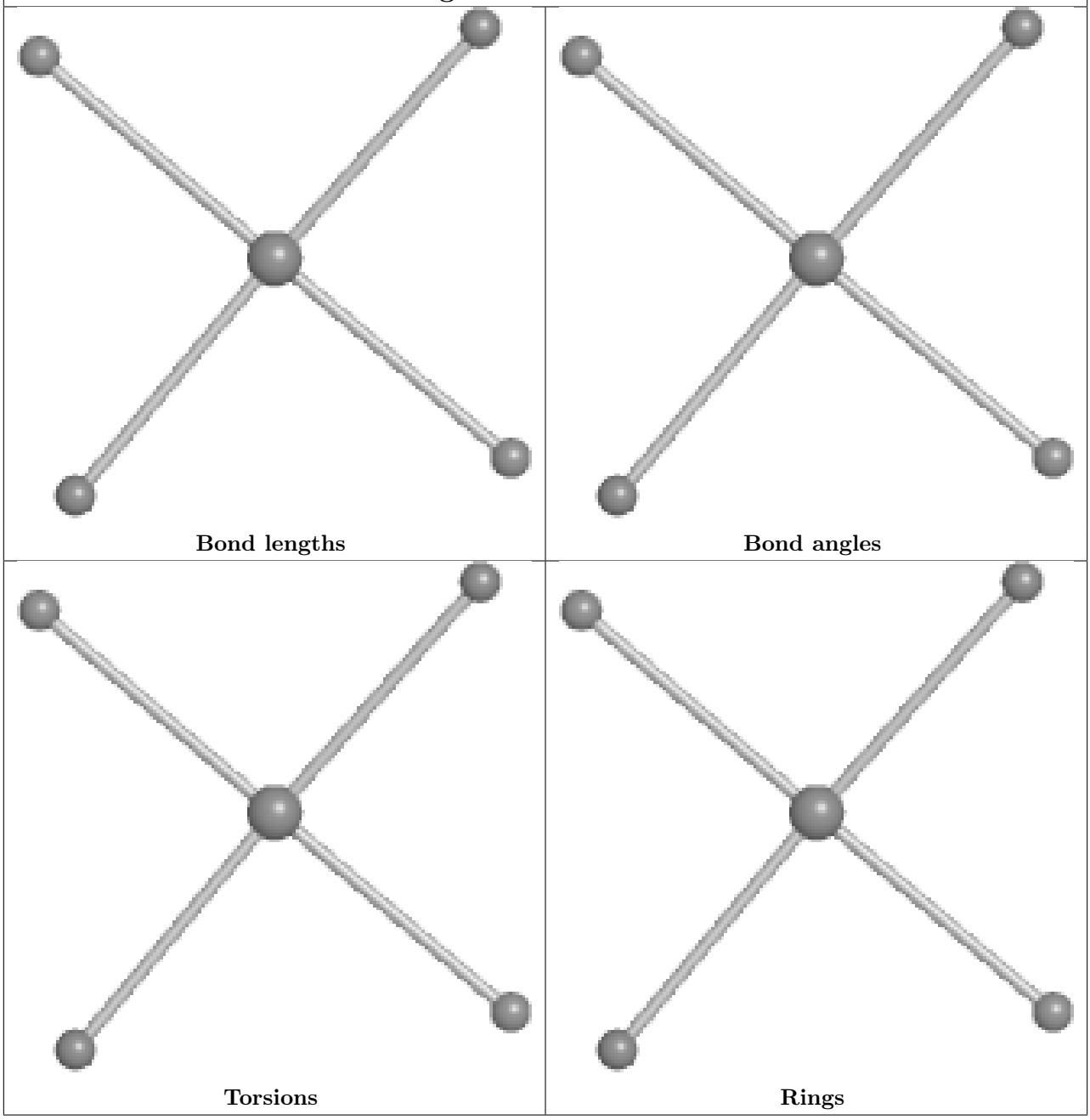


Torsions



Rings

Ligand ALF A 1003



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	442/450 (98%)	0.27	14 (3%) 50 45	68, 104, 154, 218	0
1	B	413/450 (91%)	0.40	35 (8%) 16 13	63, 97, 213, 265	0
2	C	28/29 (96%)	0.30	0 100 100	100, 137, 189, 220	0
All	All	883/929 (95%)	0.33	49 (5%) 30 26	63, 102, 194, 265	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	380	VAL	7.9
1	B	422	PRO	6.7
1	B	365	GLY	5.7
1	A	392	ARG	4.8
1	B	329	LYS	4.6
1	B	354	LEU	4.6
1	B	338	PRO	4.5
1	B	332	PHE	4.1
1	A	377	ALA	4.1
1	B	353	LEU	4.0
1	A	390	VAL	3.7
1	B	395	VAL	3.5
1	B	377	ALA	3.4
1	B	352	ILE	3.4
1	B	501	SER	3.3
1	B	363	PHE	3.1
1	A	255	GLN	3.0
1	A	258	ARG	3.0
1	B	429	LEU	2.9
1	B	328	VAL	2.9
1	B	423	VAL	2.9
1	B	391	ILE	2.8
1	A	342	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	507	LEU	2.7
1	A	89	ILE	2.7
1	B	426	ALA	2.6
1	B	294	PRO	2.5
1	B	345	LEU	2.5
1	A	294	PRO	2.5
1	A	66	GLU	2.5
1	A	373	LEU	2.5
1	B	383	LYS	2.5
1	B	330	GLY	2.4
1	B	351	VAL	2.4
1	B	382	LEU	2.4
1	B	375	ALA	2.4
1	B	253	GLU	2.4
1	B	482	TRP	2.3
1	B	343	LEU	2.3
1	B	378	LEU	2.3
1	A	482	TRP	2.3
1	A	359	LEU	2.2
1	B	349	ALA	2.2
1	B	224	LEU	2.2
1	B	369	TRP	2.2
1	B	364	ASN	2.1
1	A	322	LEU	2.1
1	B	355	ARG	2.0
1	B	386	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 oligosaccharides in this entry.

6.4 Ligands (i)

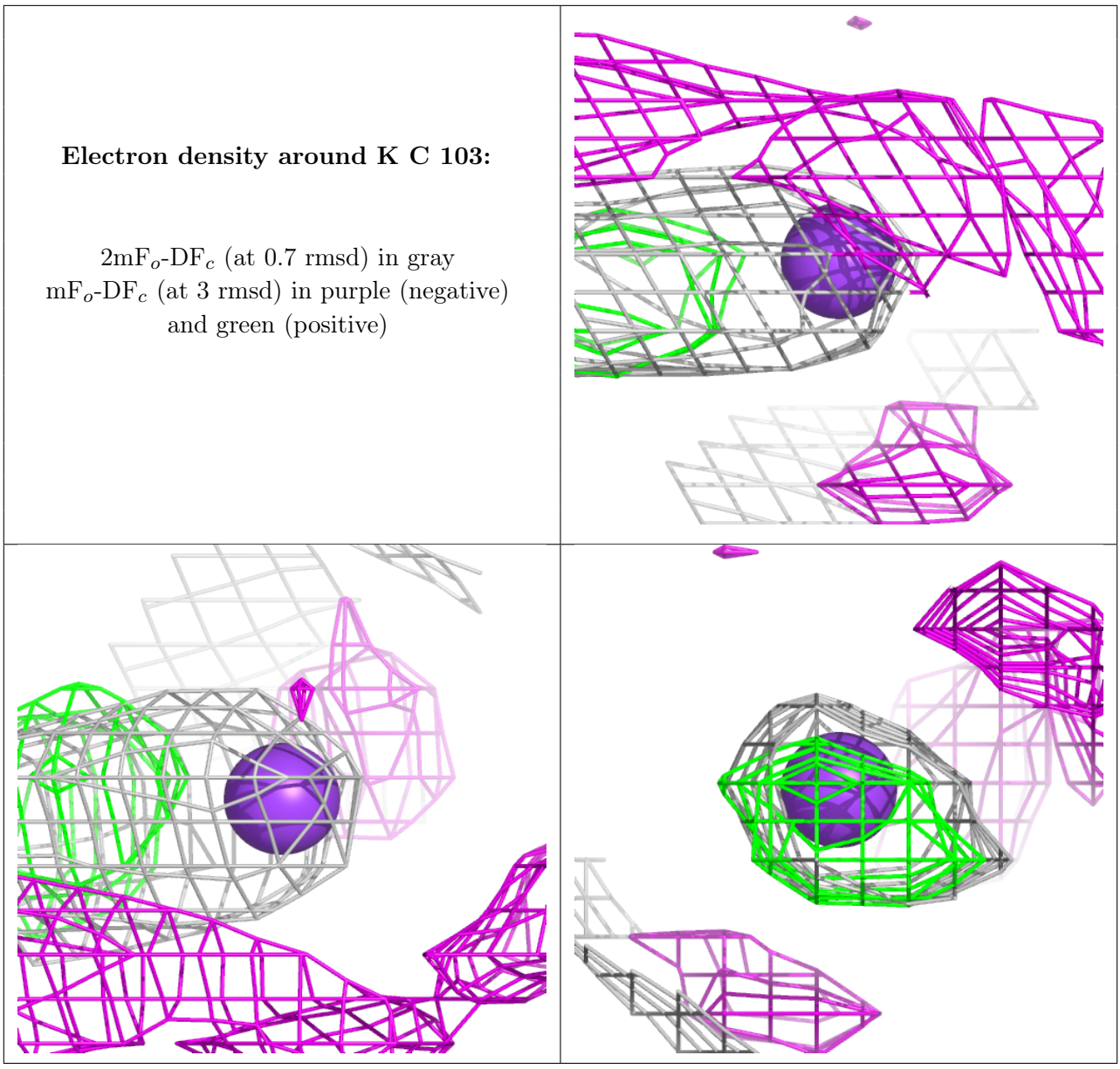
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	K	C	103	1/1	0.53	0.36	148,148,148,148	0
6	K	C	102	1/1	0.88	0.10	176,176,176,176	0
4	MG	B	1002	1/1	0.93	0.17	77,77,77,77	0
3	ADP	A	1001	27/27	0.96	0.08	61,98,114,117	0
6	K	C	101	1/1	0.97	0.09	147,147,147,147	0
3	ADP	B	1001	27/27	0.97	0.07	59,77,90,92	0
5	ALF	A	1003	5/5	0.97	0.07	81,83,88,102	0
5	ALF	B	1003	5/5	0.99	0.06	66,68,70,75	0
4	MG	A	1002	1/1	0.99	0.03	81,81,81,81	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.

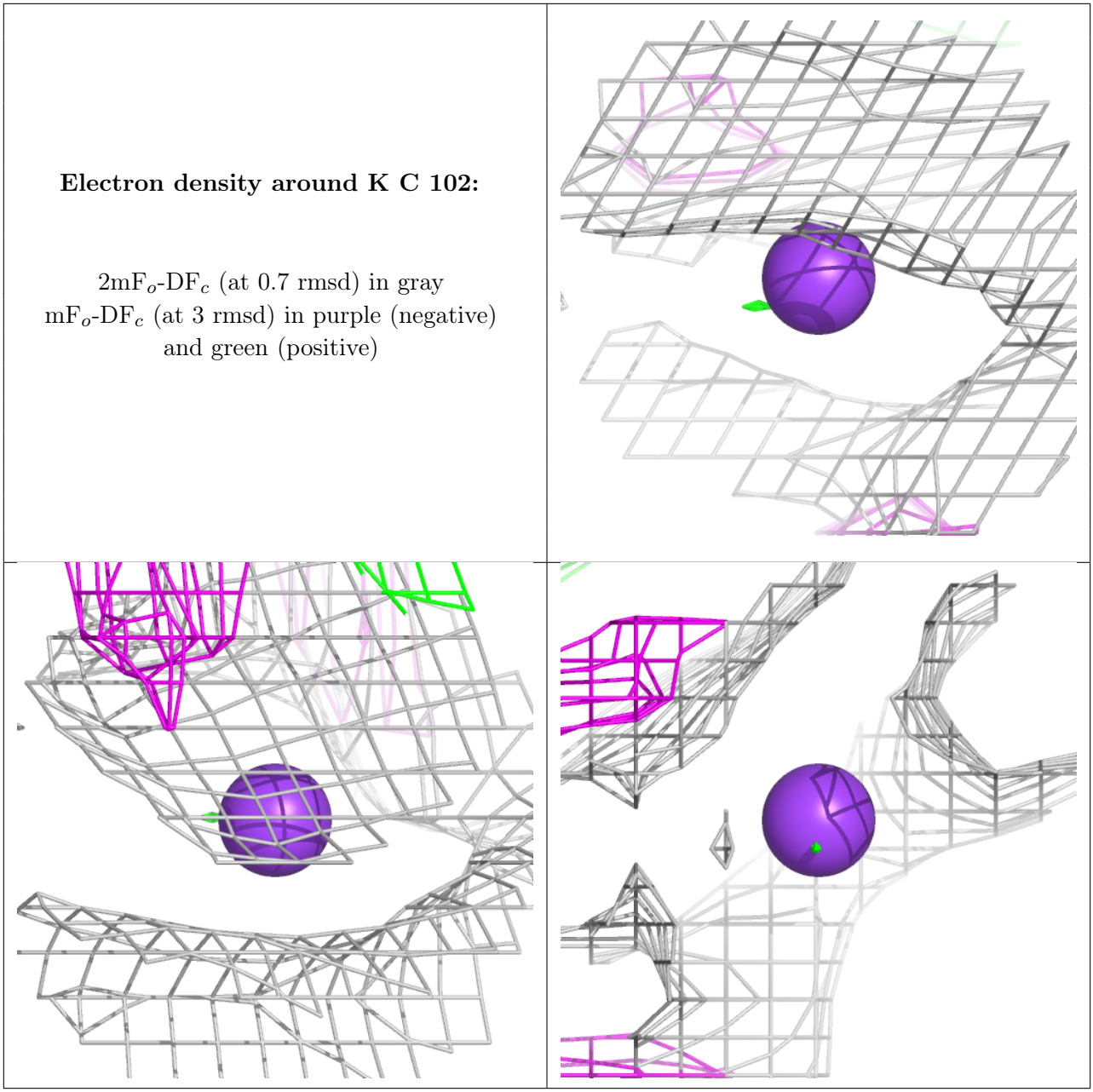
Electron density around K C 103:

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



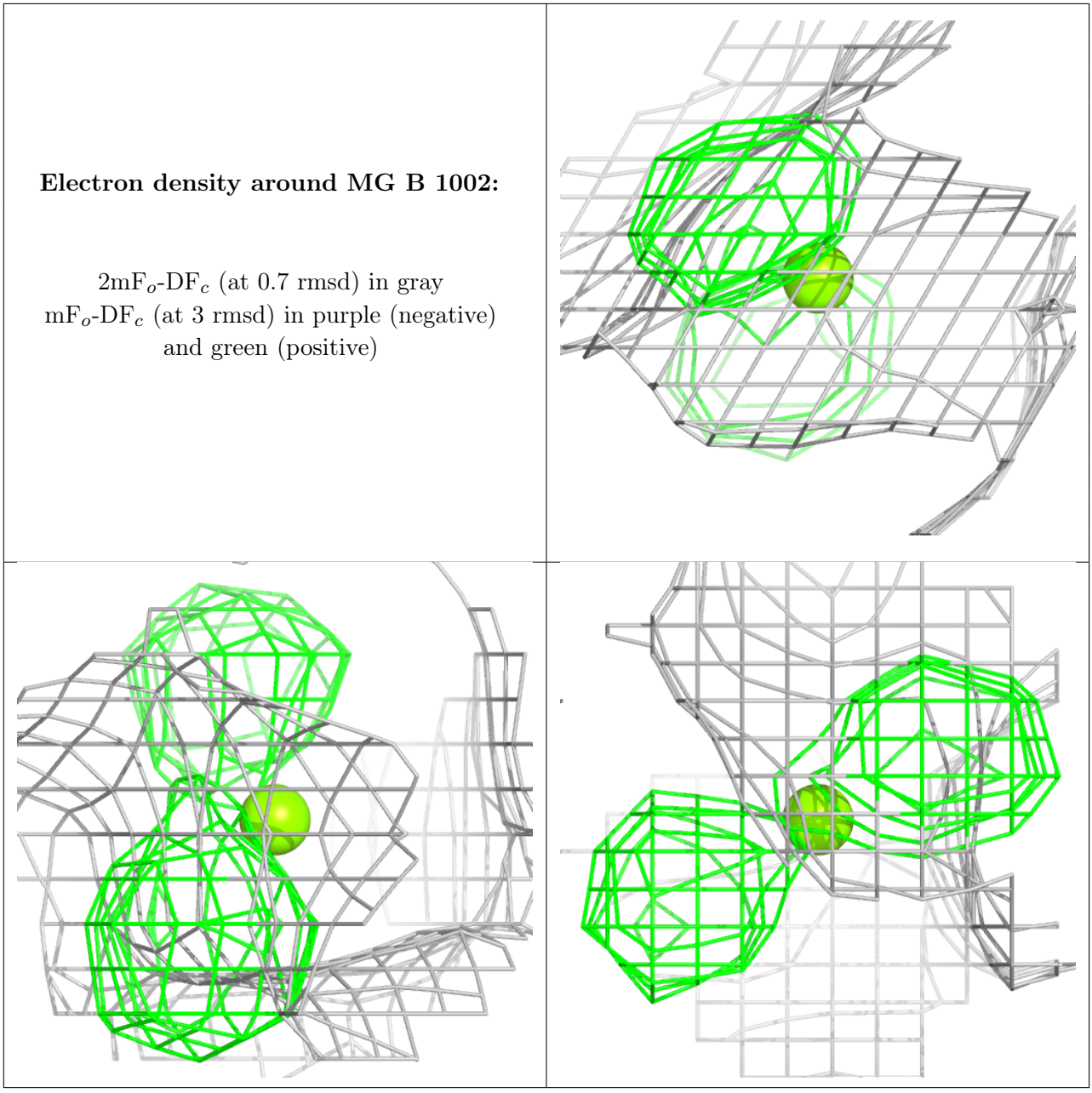
Electron density around K C 102:

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



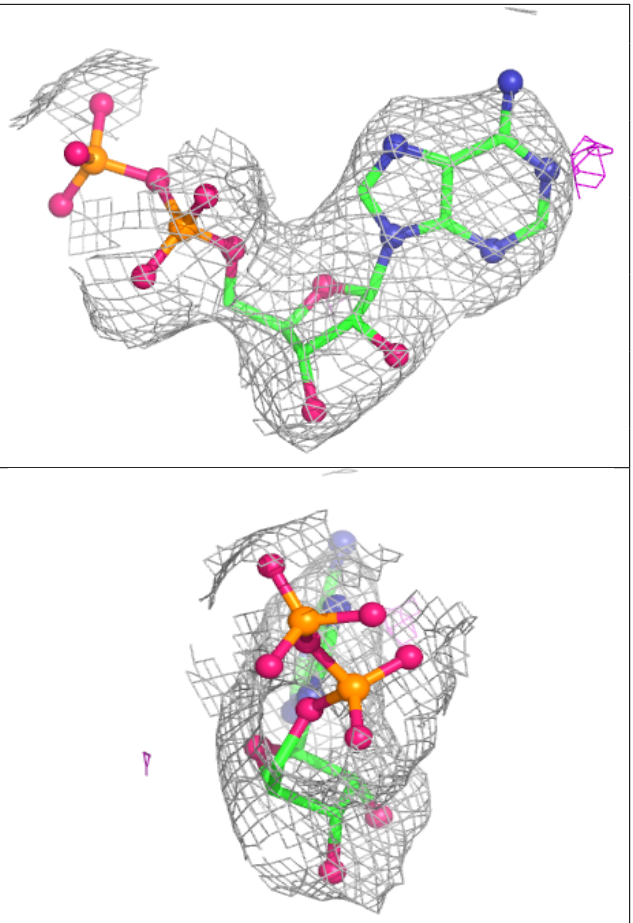
Electron density around MG B 1002:

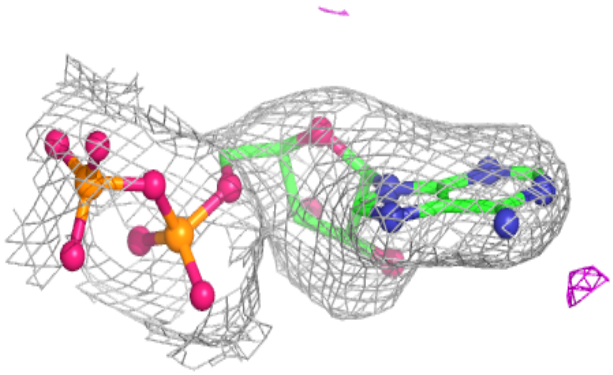
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ADP A 1001:

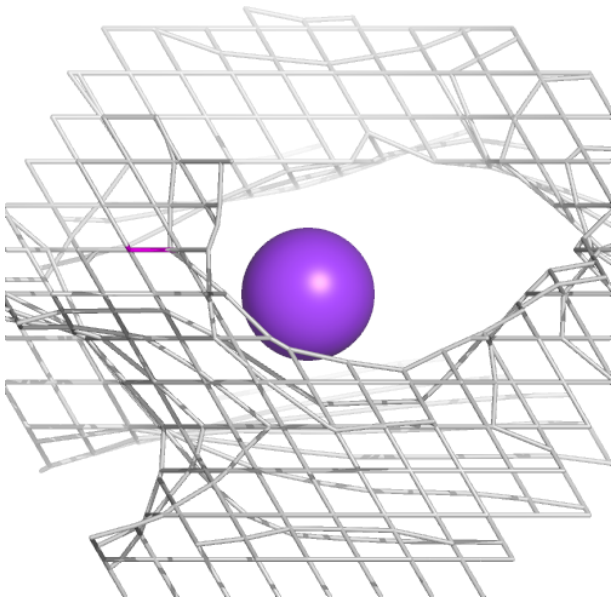
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

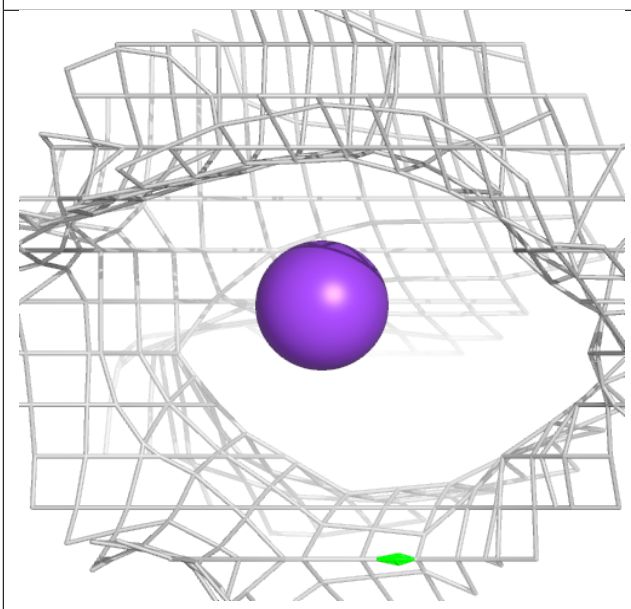


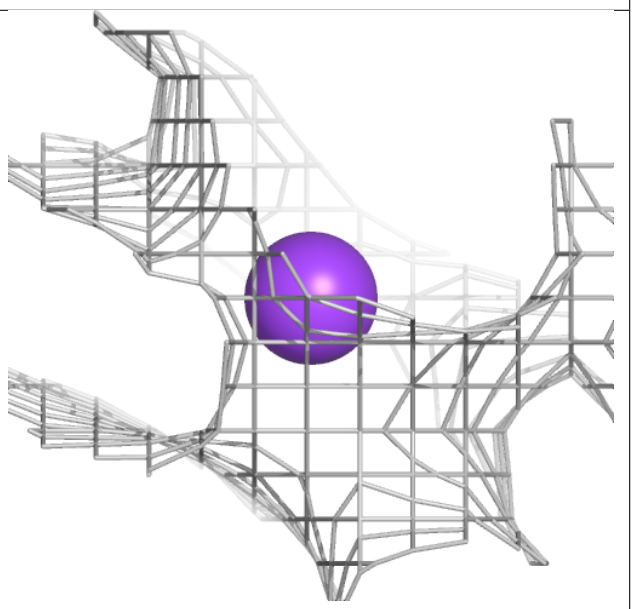


Electron density around K C 101:

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

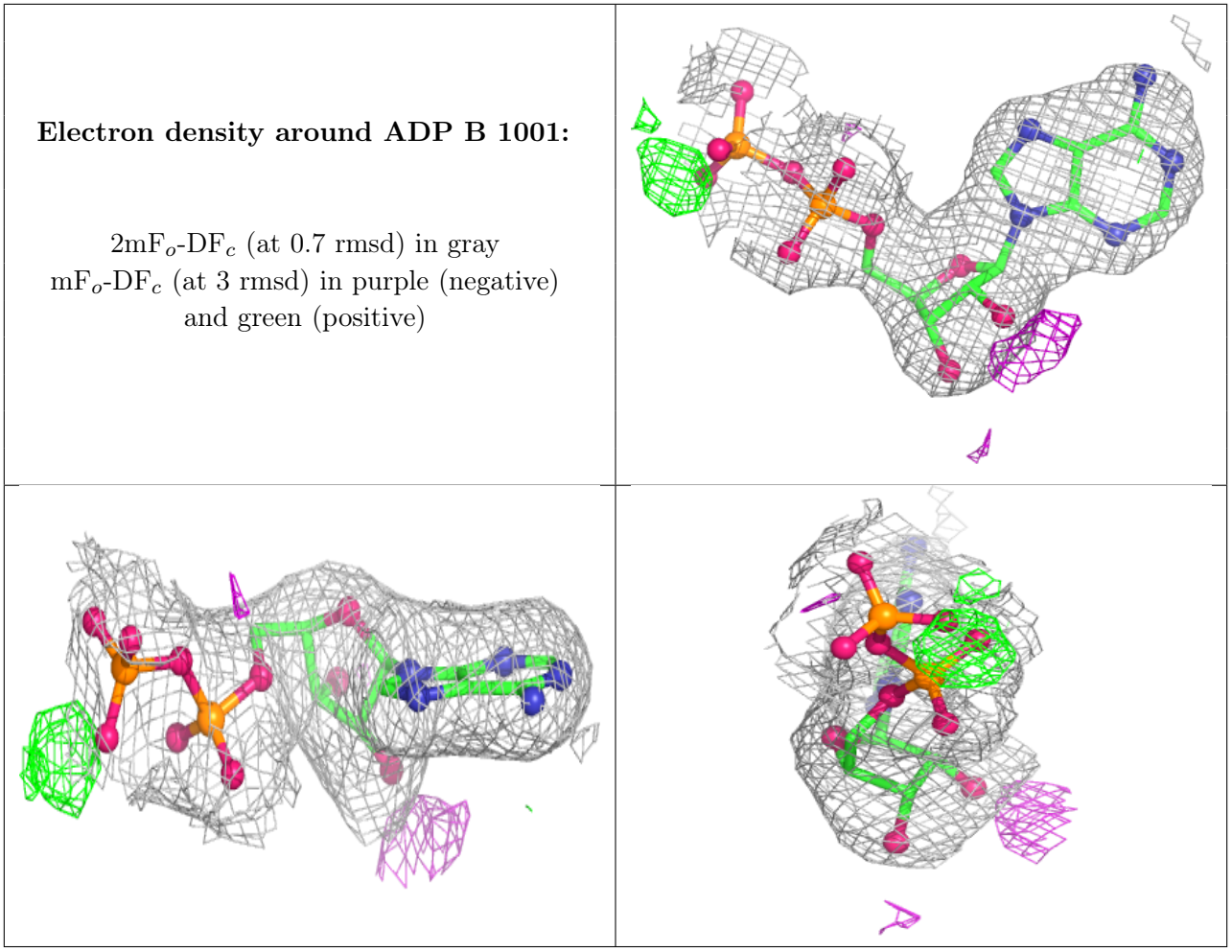






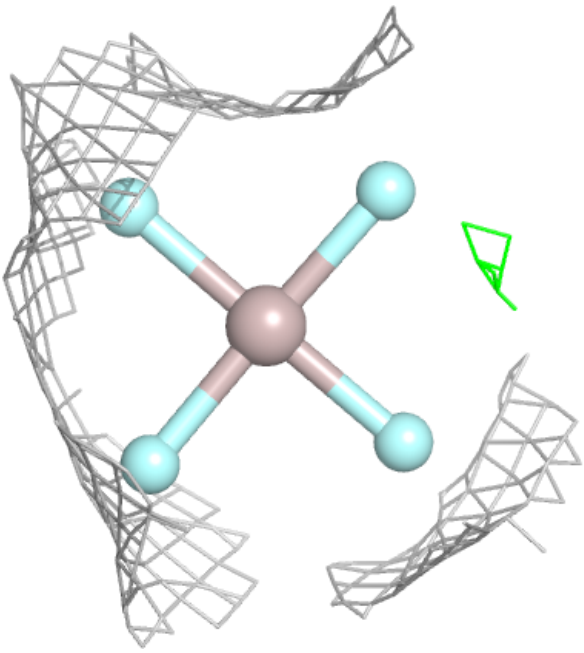
Electron density around ADP B 1001:

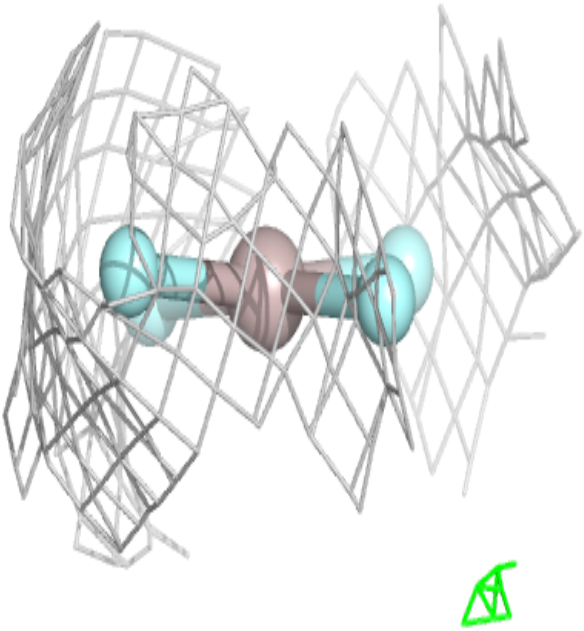
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

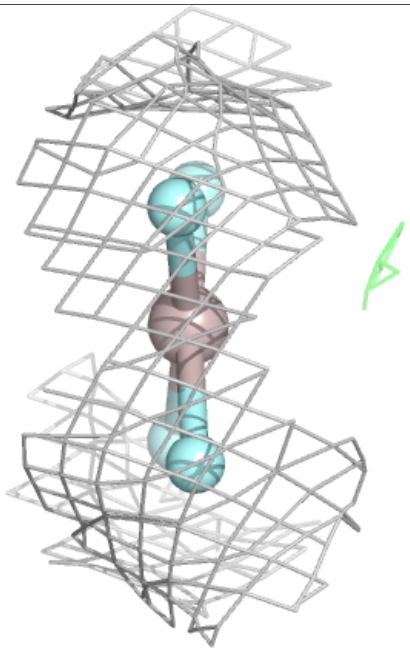


Electron density around ALF A 1003:

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

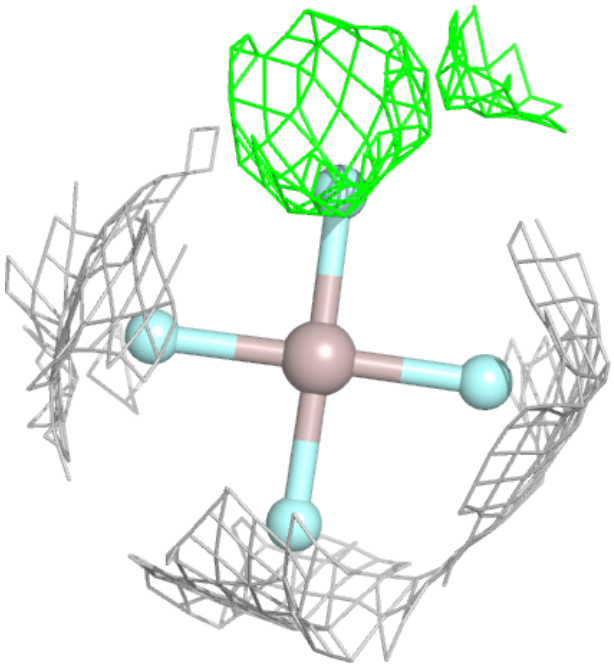


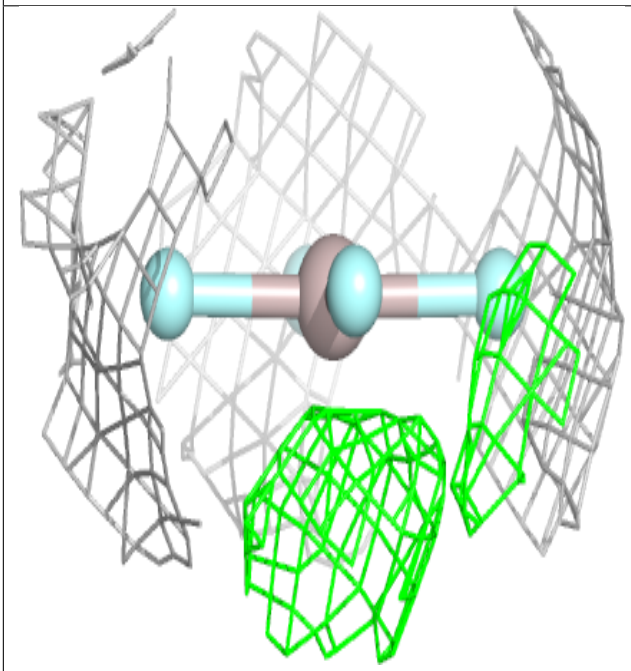


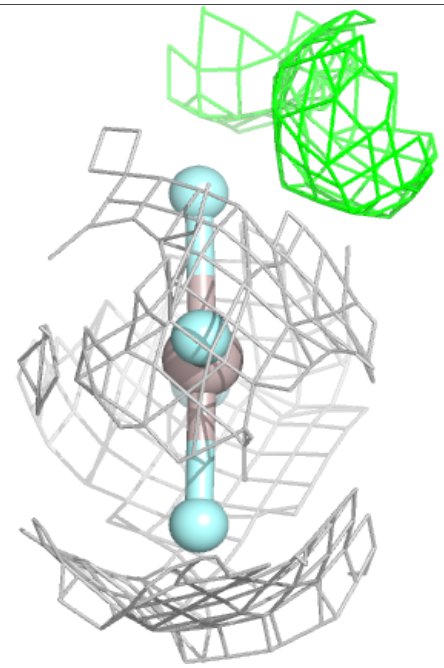


Electron density around ALF B 1003:

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

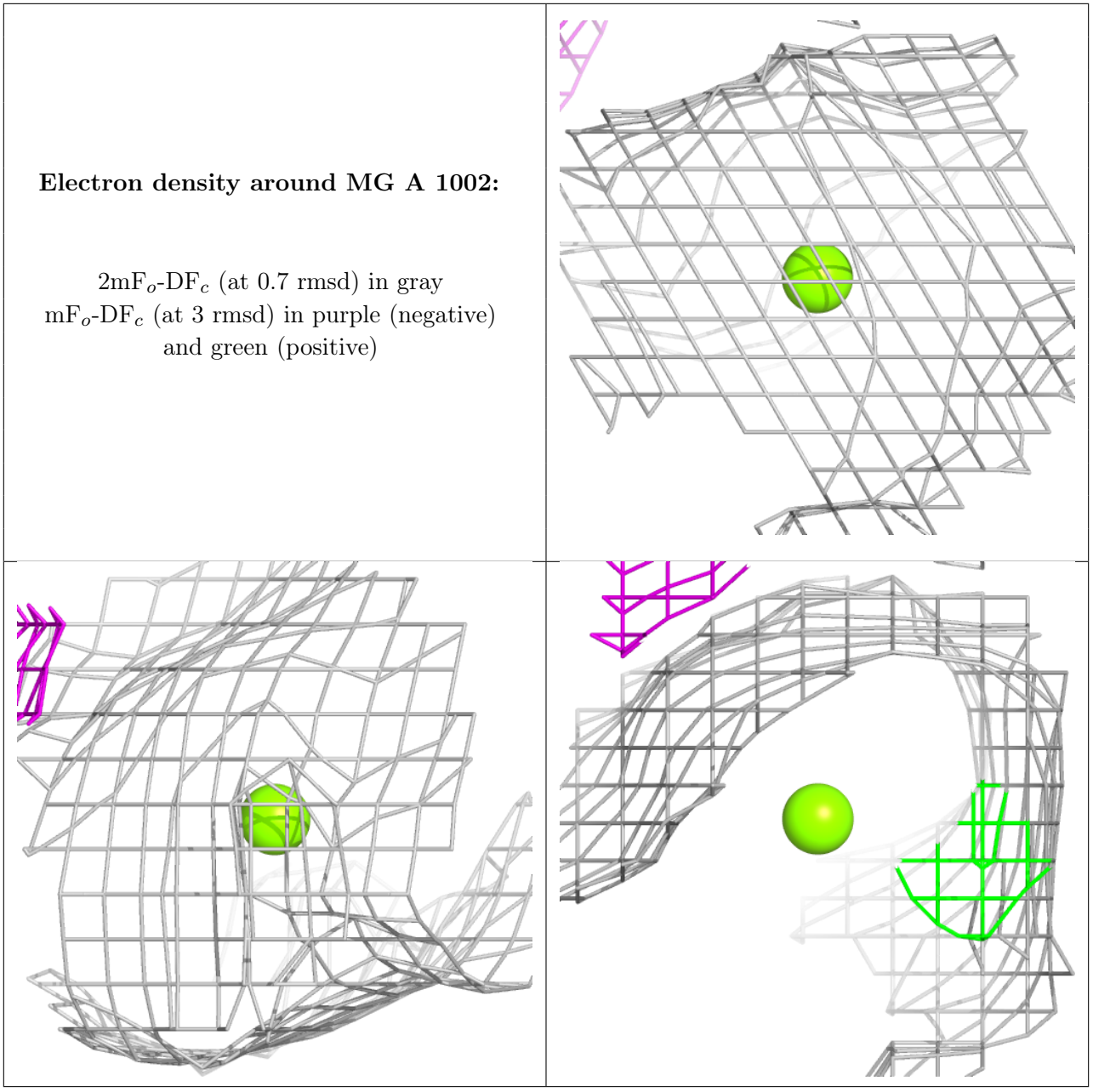






Electron density around MG A 1002:

$2mF_o$-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.