Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2022 – 06:08 pm GMT

PDB ID	:	7OAR
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 following versions of software and data (see references ⓘ) were used in the production of this report:

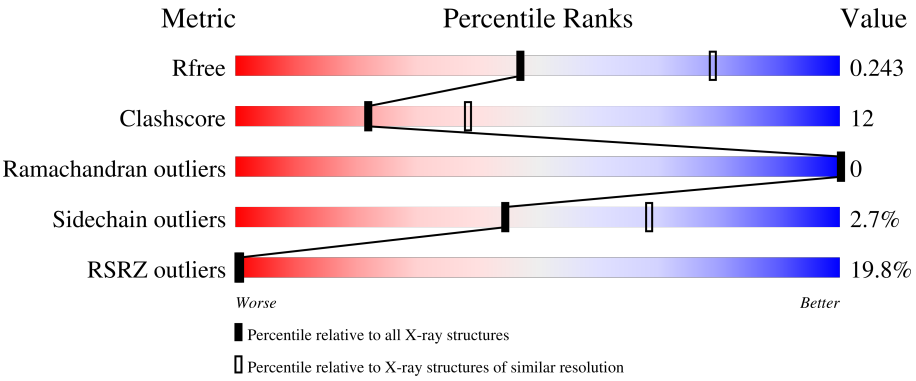
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (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	19% 76% 21%
1	B	450	17% 68% 21% 8%
2	C	29	45% 86% 10%

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.

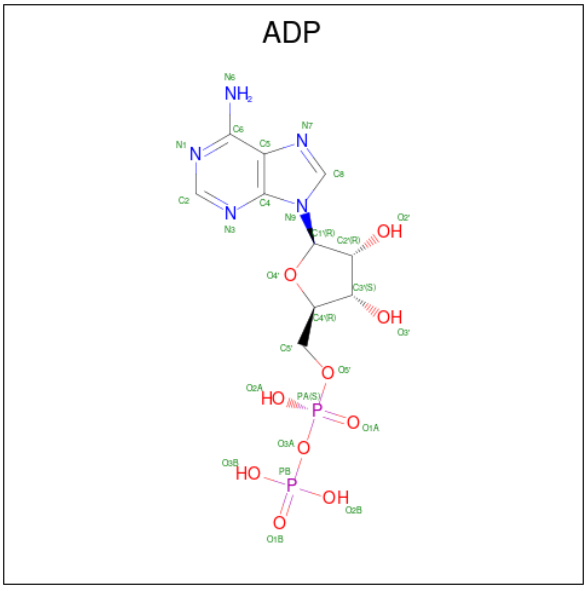
- Molecule 1 is a protein called Pif1 helicase.

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 (three-letter code: 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		

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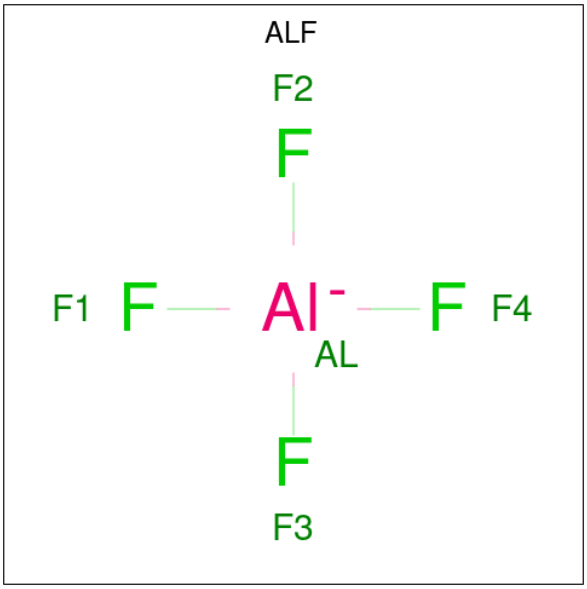
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: 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 (three-letter code: 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 (three-letter code: 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.

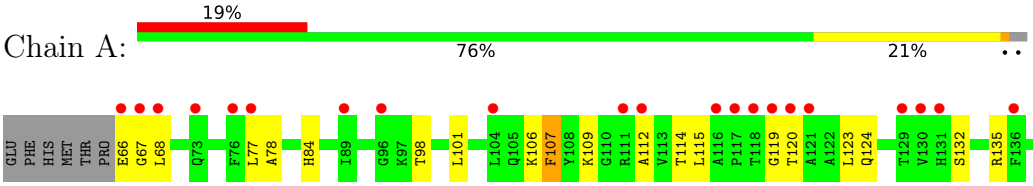
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	17	Total O 17 17	0	0
7	B	21	Total O 21 21	0	0

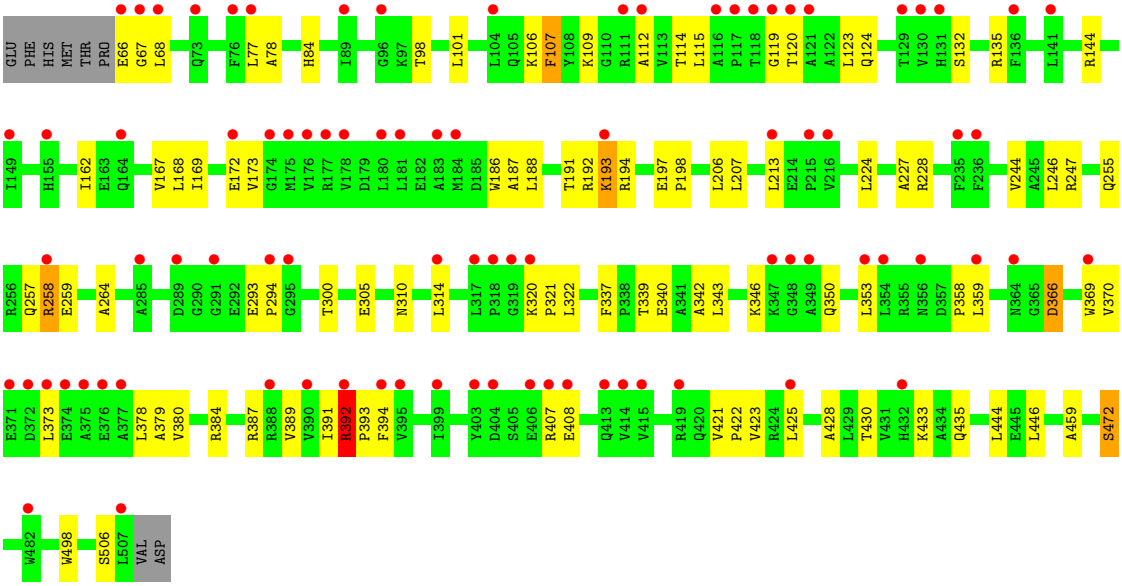
3 Residue-property plots (i)

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

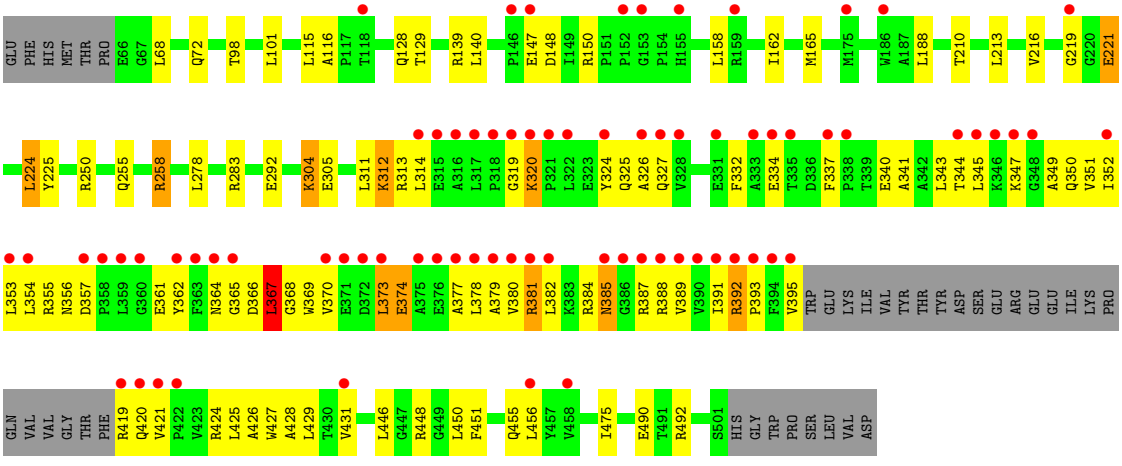
Chain A:



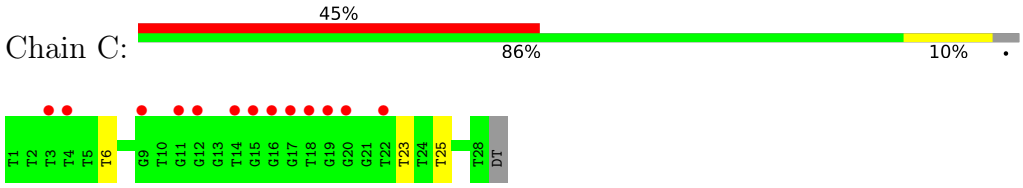


• Molecule 1: Pif1 helicase

Chain B:



• Molecule 2: DNA (28-MER)



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 37.59 – 2.58	Depositor EDS
% Data completeness (in resolution range)	93.6 (37.39-2.58) 93.6 (37.59-2.58)	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 0.194 , 0.243	Depositor DCC
R_{free} test set	2130 reflections (4.78%)	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)	(Not available) , (Not available)	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, MG, ALF, ADP

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	0.43	1/3638 (0.0%)	0.64	2/4938 (0.0%)
1	B	0.43	0/3379	0.68	4/4582 (0.1%)
2	C	0.82	0/630	1.13	0/977
All	All	0.48	1/7647 (0.0%)	0.71	6/10497 (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	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	8.73	1.50	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	367	LEU	CA-CB-CG	7.39	132.29	115.30
1	B	224	LEU	CA-CB-CG	6.24	129.65	115.30
1	B	224	LEU	CB-CG-CD2	-6.00	100.80	111.00
1	A	193	LYS	CA-CB-CG	5.45	125.40	113.40
1	A	66	GLU	C-N-CA	-5.41	110.94	122.30
1	B	373	LEU	CA-CB-CG	-5.21	103.33	115.30

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	77	0
1	B	3304	0	3376	96	0
2	C	565	0	313	3	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	173	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 (173) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ASP:HB3	1:B:362:TYR:CZ	2.20	0.77
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: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: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:392:ARG:C	1:A:392:ARG:HD2	2.20	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: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:B:162:ILE:HA	1:B:165:MET:HE3	1.86	0.58
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

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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:369:TRP:C	1:A:380:VAL:HG23	2.26	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: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: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: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:B:352:ILE:HD11	1:B:365:GLY:C	2.31	0.51
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:340:GLU:H	1:B:340:GLU:CD	2.15	0.50
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
1:A:187:ALA:O	1:A:191:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:VAL:HG12	1:A:391:ILE:HD13	1.94	0.49
1:B:392:ARG:HD3	1:B:392:ARG:C	2.33	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
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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:107:PHE:CD1	1:A:107:PHE:C	2.93	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:352:ILE:HG13	1:B:366:ASP:C	2.41	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	360 (98%)	9 (2%)	49	72
1	B	342/377 (91%)	332 (97%)	10 (3%)	42	66
All	All	711/754 (94%)	692 (97%)	19 (3%)	44	68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	PHE
1	A	132	SER
1	A	135	ARG
1	A	258	ARG
1	A	359	LEU
1	A	366	ASP
1	A	387	ARG
1	A	392	ARG
1	A	472	SER
1	B	250	ARG
1	B	258	ARG
1	B	304	LYS
1	B	312	LYS
1	B	332	PHE
1	B	367	LEU
1	B	381	ARG
1	B	385	ASN
1	B	392	ARG
1	B	492	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	GLN
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 monosaccharides 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	$\#\|Z\| > 2$
5	ALF	B	1003	-	0,4,4	-	-	-		
5	ALF	A	1003	-	0,4,4	-	-	-		
3	ADP	A	1001	4	24,29,29	0.92	1 (4%)	29,45,45	1.47	5 (17%)
3	ADP	B	1001	4	24,29,29	1.24	2 (8%)	29,45,45	1.43	5 (17%)

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	A	1001	4	-	4/12/32/32	0/3/3/3
3	ADP	B	1001	4	-	2/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	ADP	PB-O3B	-2.88	1.43	1.54
3	B	1001	ADP	C5-C4	2.62	1.47	1.40
3	A	1001	ADP	C5-C4	2.53	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1001	ADP	C4-C5-N7	-3.66	105.58	109.40
3	A	1001	ADP	N3-C2-N1	-3.41	123.35	128.68
3	B	1001	ADP	O3'-C3'-C4'	-2.76	103.07	111.05
3	B	1001	ADP	N3-C2-N1	-2.57	124.65	128.68
3	A	1001	ADP	C2-N1-C6	2.56	123.13	118.75
3	A	1001	ADP	C4-C5-N7	-2.40	106.90	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	B	1001	ADP	C5-C6-N6	2.17	123.65	120.35
3	B	1001	ADP	C2-N1-C6	2.03	122.23	118.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

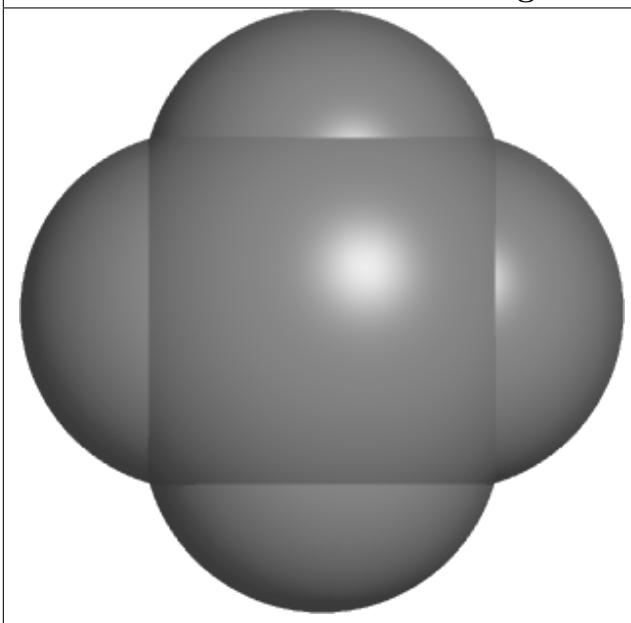
Mol	Chain	Res	Type	Atoms
3	A	1001	ADP	C5'-O5'-PA-O2A
3	B	1001	ADP	PA-O3A-PB-O2B
3	A	1001	ADP	C5'-O5'-PA-O3A
3	A	1001	ADP	C5'-O5'-PA-O1A
3	A	1001	ADP	O4'-C4'-C5'-O5'
3	B	1001	ADP	PA-O3A-PB-O1B

There are no ring outliers.

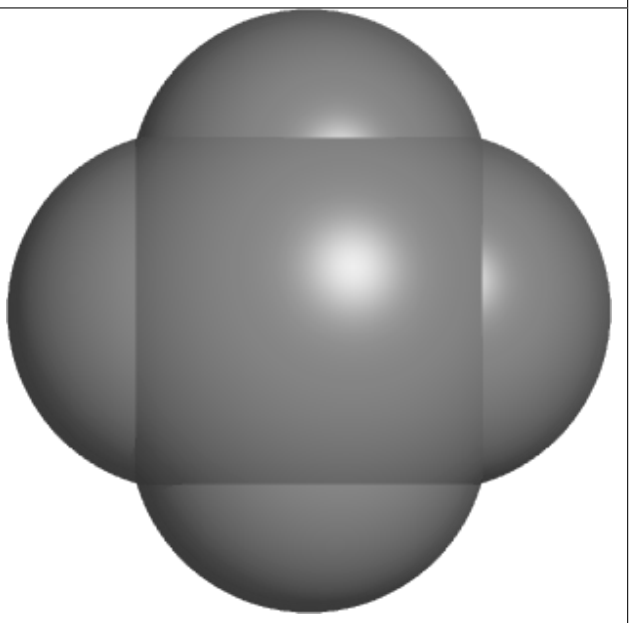
No monomer is involved in short contacts.

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.

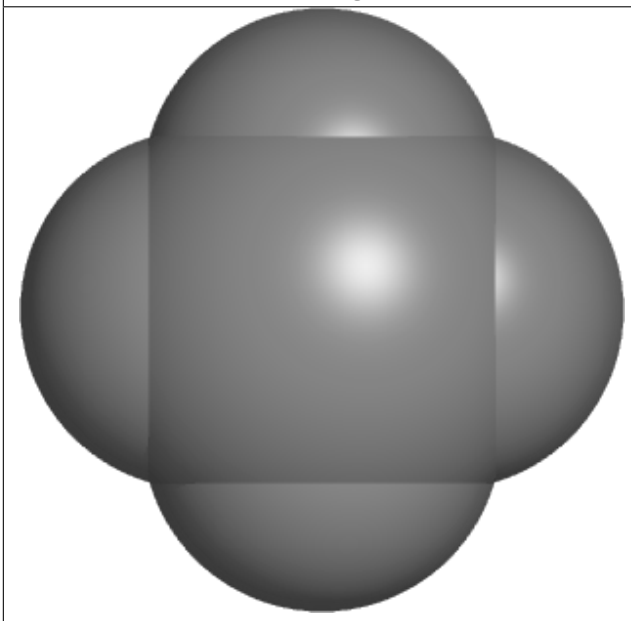
Ligand ALF B 1003



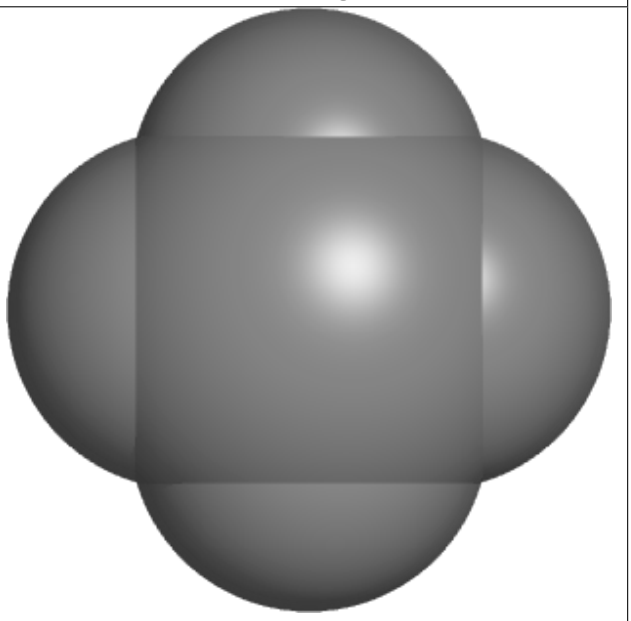
Bond lengths



Bond angles

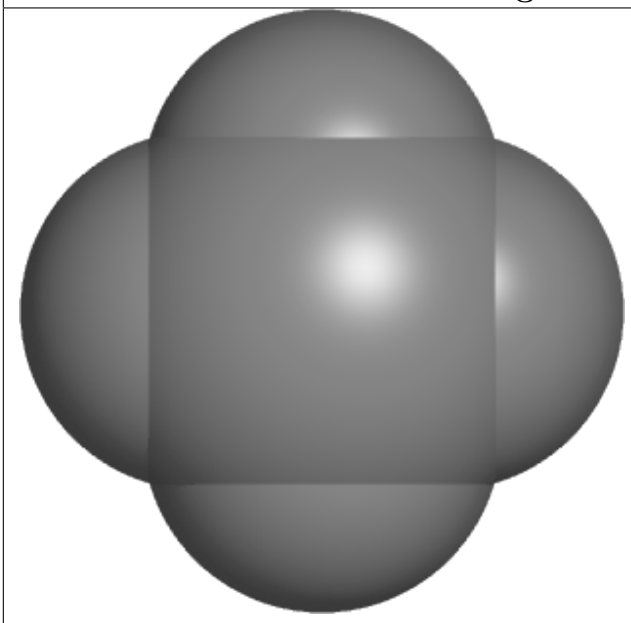


Torsions

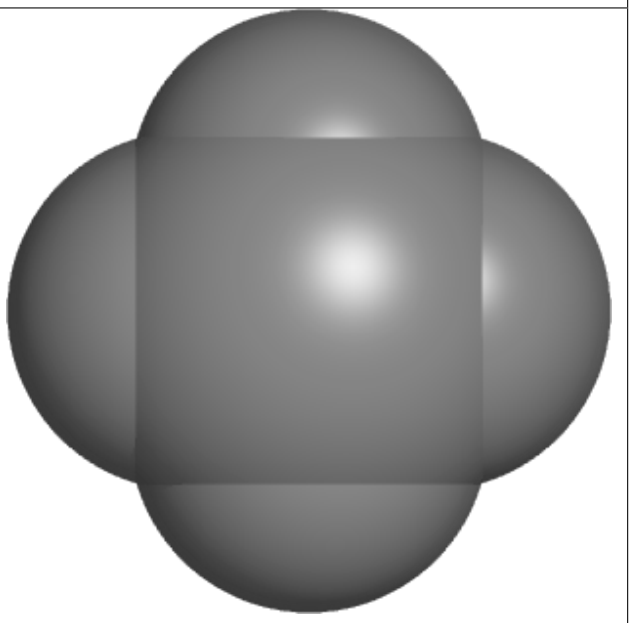


Rings

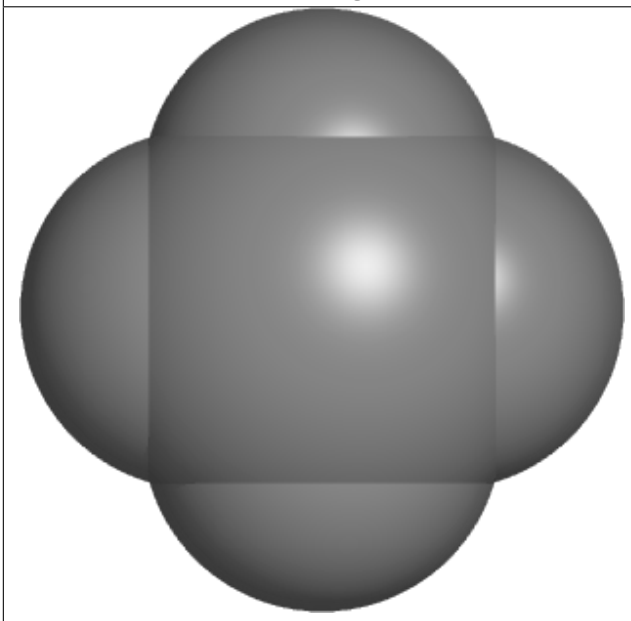
Ligand ALF A 1003



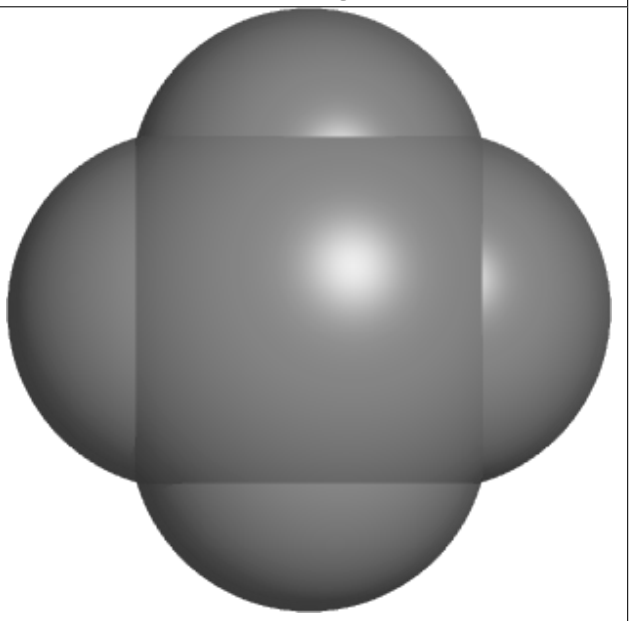
Bond lengths



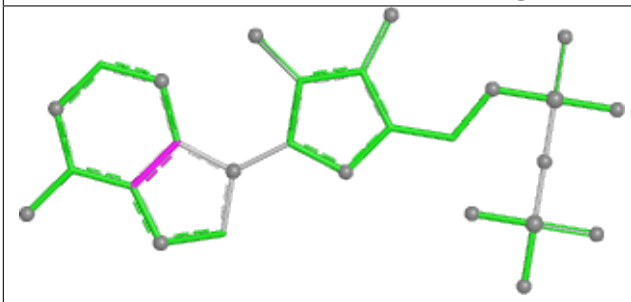
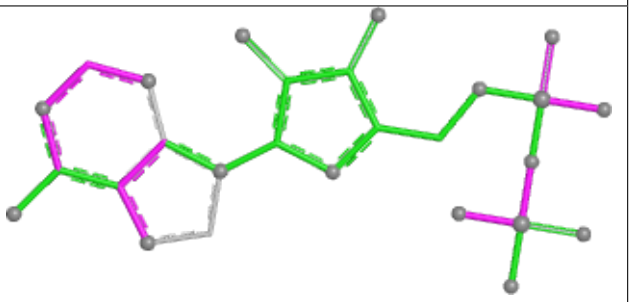
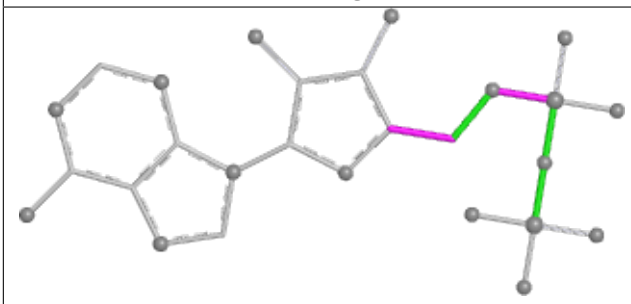
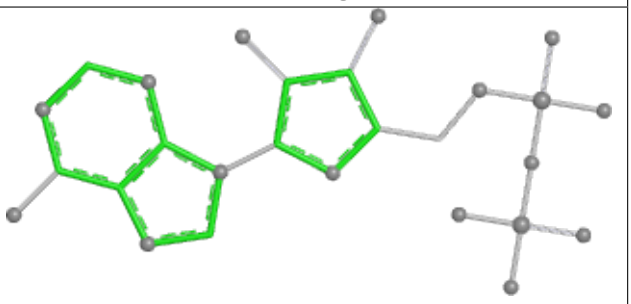
Bond angles

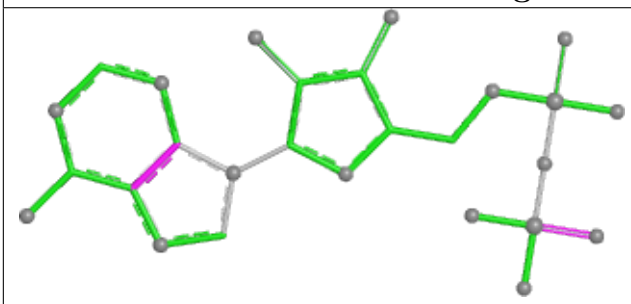
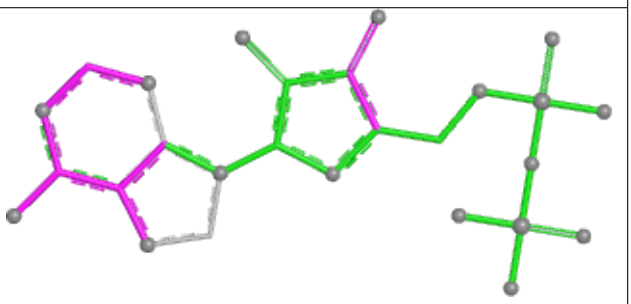
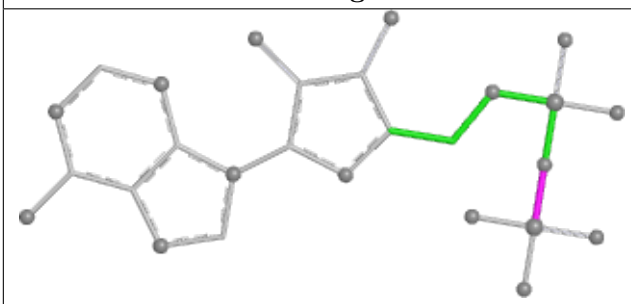
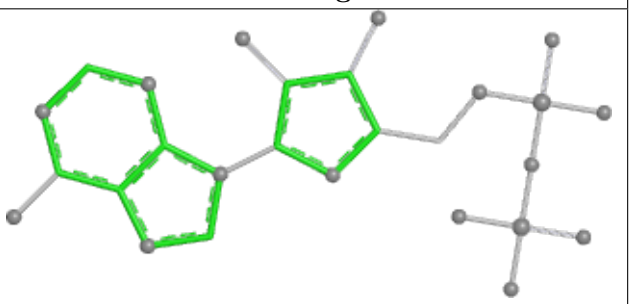


Torsions



Rings

Ligand ADP A 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

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%)	0.95	87 (19%)	1	0	68, 104, 154, 218	0
1	B	413/450 (91%)	1.24	75 (18%)	1	1	63, 97, 213, 265	0
2	C	28/29 (96%)	1.83	13 (46%)	0	0	100, 137, 189, 220	0
All	All	883/929 (95%)	1.11	175 (19%)	1	0	63, 102, 194, 265	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	ALA	18.8
1	B	380	VAL	15.3
1	B	378	LEU	12.5
1	B	422	PRO	12.2
1	B	219	GLY	10.1
1	A	377	ALA	10.1
1	B	359	LEU	9.2
1	B	386	GLY	9.1
1	A	66	GLU	9.0
1	B	391	ILE	8.6
1	B	370	VAL	8.0
1	B	354	LEU	7.8
1	B	335	THR	7.6
1	B	318	PRO	7.6
1	B	372	ASP	6.9
1	B	376	GLU	6.7
1	B	317	LEU	6.6
1	B	328	VAL	6.4
1	B	381	ARG	6.3
1	A	294	PRO	6.3
1	B	389	VAL	6.2
2	C	15	DG	5.6
1	A	318	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	314	LEU	5.4
1	B	382	LEU	5.2
1	A	174	GLY	5.2
1	B	314	LEU	5.0
1	B	390	VAL	5.0
1	B	387	ARG	4.9
1	B	388	ARG	4.9
1	B	385	ASN	4.9
1	A	175	MET	4.7
1	A	392	ARG	4.5
1	B	360	GLY	4.4
1	A	408	GLU	4.4
1	B	395	VAL	4.4
1	B	327	GLN	4.3
1	B	420	GLN	4.2
1	B	345	LEU	4.2
1	B	331	GLU	4.2
1	A	317	LEU	4.2
2	C	18	DT	4.2
1	A	67	GLY	4.1
1	B	326	ALA	4.1
1	B	375	ALA	4.1
1	A	413	GLN	4.1
1	A	289	ASP	4.1
1	B	338	PRO	4.0
1	B	379	ALA	4.0
1	A	181	LEU	4.0
1	A	373	LEU	3.9
1	A	348	GLY	3.9
1	B	334	GLU	3.9
1	B	393	PRO	3.9
1	B	421	VAL	3.9
1	B	394	PHE	3.9
1	A	258	ARG	3.9
1	B	373	LEU	3.8
1	A	131	HIS	3.8
1	B	322	LEU	3.8
1	A	120	THR	3.8
1	A	295	GLY	3.7
1	B	364	ASN	3.6
1	B	371	GLU	3.6
1	A	213	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	119	GLY	3.6
1	B	392	ARG	3.5
1	A	141	LEU	3.5
2	C	14	DT	3.5
1	B	365	GLY	3.5
2	C	11	DG	3.5
1	A	73	GLN	3.5
1	A	129	THR	3.5
1	A	347	LYS	3.4
1	A	193	LYS	3.4
2	C	16	DG	3.4
1	A	155	HIS	3.4
1	B	353	LEU	3.4
1	B	316	ALA	3.4
1	A	215	PRO	3.4
2	C	12	DG	3.3
1	A	116	ALA	3.3
1	B	153	GLY	3.3
1	A	371	GLU	3.2
1	B	319	GLY	3.1
1	A	407	ARG	3.1
1	A	117	PRO	3.1
1	B	146	PRO	3.0
1	A	176	VAL	3.0
1	A	291	GLY	3.0
1	A	285	ALA	3.0
1	B	357	ASP	3.0
1	A	364	ASN	2.9
1	B	321	PRO	2.9
1	A	136	PHE	2.9
1	A	320	LYS	2.9
2	C	4	DT	2.9
1	A	399	ILE	2.8
1	B	419	ARG	2.8
2	C	19	DG	2.8
1	A	432	HIS	2.8
1	B	363	PHE	2.8
1	B	333	ALA	2.8
1	A	319	GLY	2.8
1	B	147	GLU	2.8
1	B	458	VAL	2.7
1	A	77	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	375	ALA	2.7
1	A	89	ILE	2.7
1	A	404	ASP	2.7
1	A	180	LEU	2.7
1	B	456	LEU	2.7
1	A	388	ARG	2.7
1	A	184	MET	2.7
1	A	507	LEU	2.6
1	A	68	LEU	2.6
1	A	216	VAL	2.6
1	A	369	TRP	2.6
1	A	372	ASP	2.6
1	A	354	LEU	2.5
1	A	112	ALA	2.5
1	A	111	ARG	2.5
1	A	76	PHE	2.5
2	C	17	DG	2.5
1	A	183	ALA	2.5
1	A	403	TYR	2.5
1	A	353	LEU	2.5
1	B	347	LYS	2.5
1	A	149	ILE	2.5
1	A	406	GLU	2.5
1	B	320	LYS	2.5
1	B	152	PRO	2.5
1	A	104	LEU	2.4
1	B	348	GLY	2.4
1	A	482	TRP	2.4
1	A	394	PHE	2.4
1	A	118	THR	2.4
1	B	358	PRO	2.4
1	A	359	LEU	2.4
1	A	390	VAL	2.4
1	B	352	ILE	2.4
1	A	172	GLU	2.4
1	B	315	GLU	2.4
1	A	349	ALA	2.4
1	B	159	ARG	2.4
2	C	3	DT	2.4
1	A	164	GLN	2.3
1	A	376	GLU	2.3
1	B	186	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	175	MET	2.3
1	B	118	THR	2.3
1	A	419	ARG	2.3
1	A	121	ALA	2.3
1	A	130	VAL	2.3
1	A	374	GLU	2.3
1	B	324	TYR	2.3
1	A	178	VAL	2.2
1	A	395	VAL	2.2
1	A	425	LEU	2.2
2	C	20	DG	2.2
1	B	362	TYR	2.2
1	A	414	VAL	2.2
1	A	236	PHE	2.2
2	C	9	DG	2.2
1	B	431	VAL	2.1
1	A	96	GLY	2.1
1	A	356	ASN	2.1
1	B	344	THR	2.1
2	C	22	DT	2.1
1	A	177	ARG	2.1
1	B	155	HIS	2.0
1	B	337	PHE	2.0
1	B	346	LYS	2.0
1	A	415	VAL	2.0
1	A	235	PHE	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)

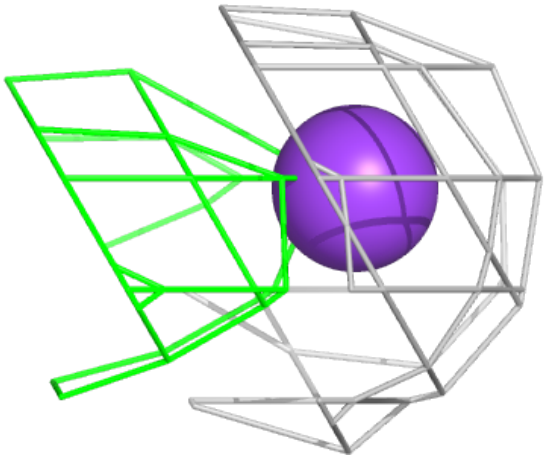
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

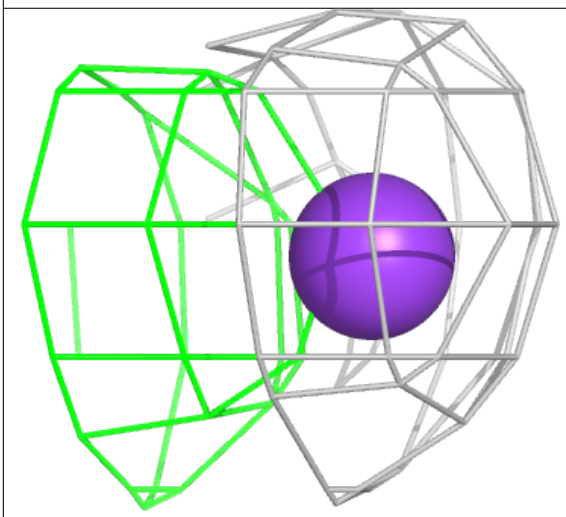
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	K	C	103	1/1	0.20	0.27	148,148,148,148	0
6	K	C	102	1/1	0.55	0.10	176,176,176,176	0
3	ADP	A	1001	27/27	0.91	0.18	61,98,114,117	0
4	MG	A	1002	1/1	0.92	0.11	81,81,81,81	0
4	MG	B	1002	1/1	0.93	0.23	77,77,77,77	0
6	K	C	101	1/1	0.93	0.15	147,147,147,147	0
3	ADP	B	1001	27/27	0.97	0.18	59,77,90,92	0
5	ALF	B	1003	5/5	0.98	0.17	66,68,70,75	0
5	ALF	A	1003	5/5	0.98	0.22	81,83,88,102	0

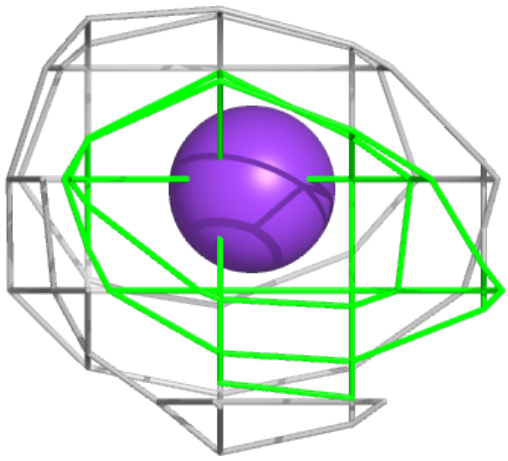
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

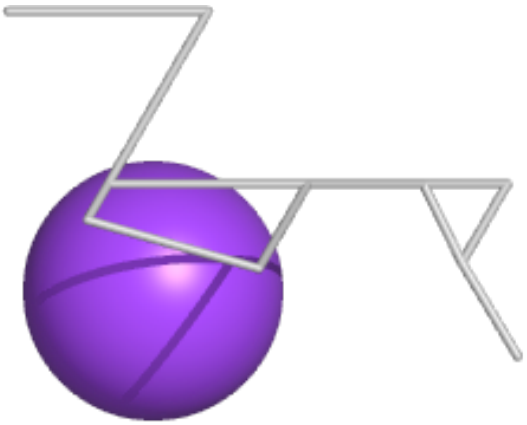


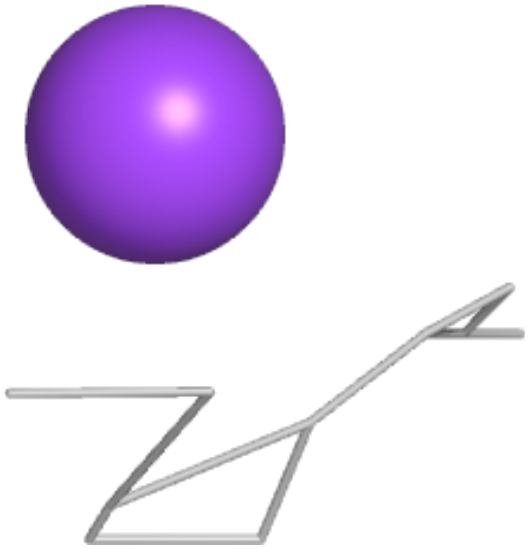


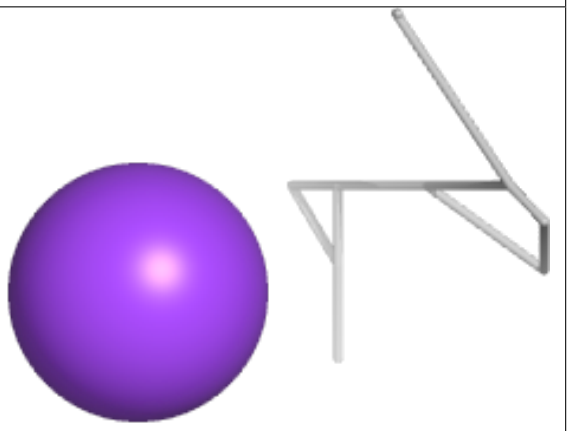


Electron density around K C 102:

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

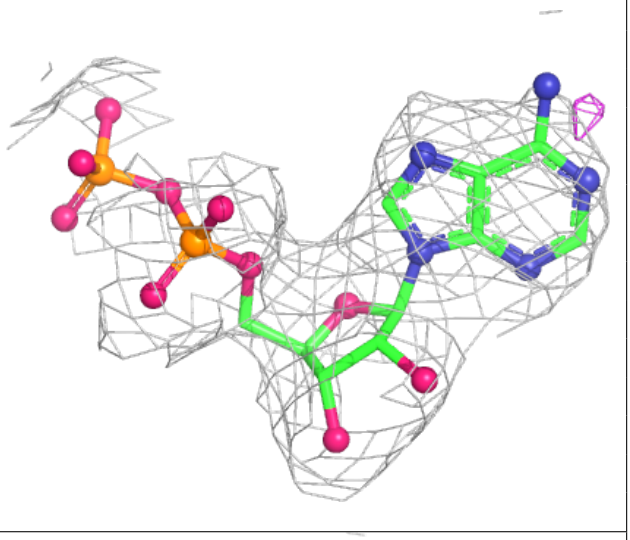


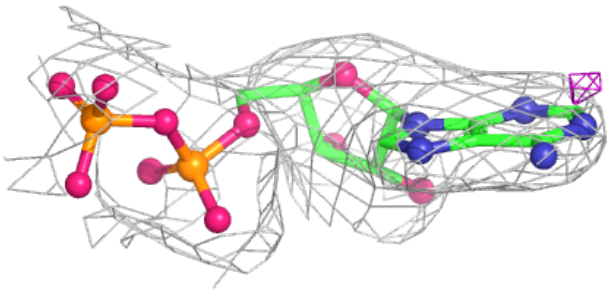


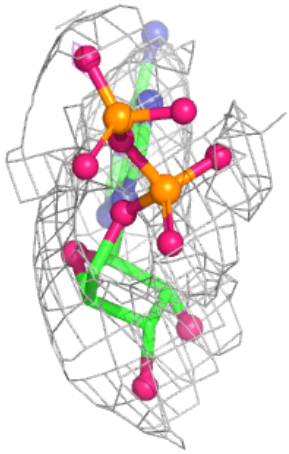


Electron density around ADP A 1001:

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

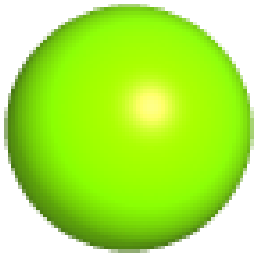


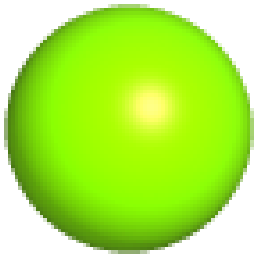


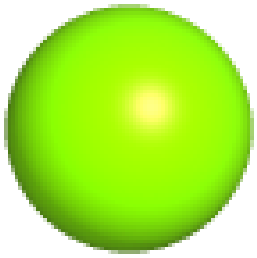


Electron density around MG A 1002:

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

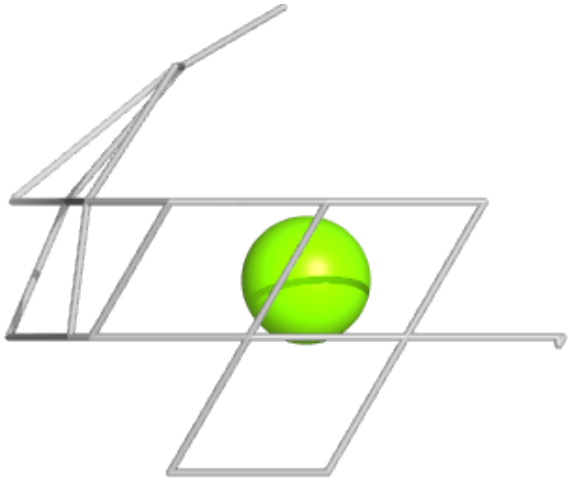


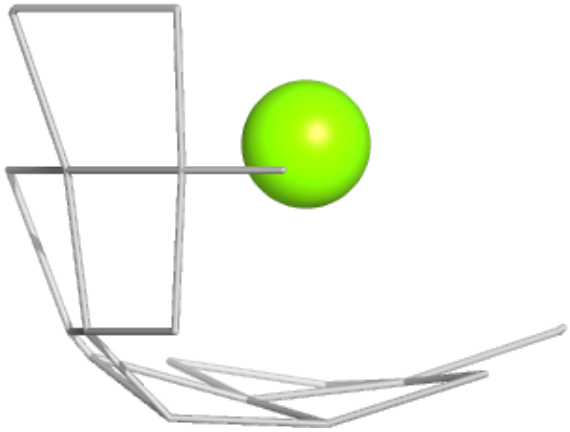


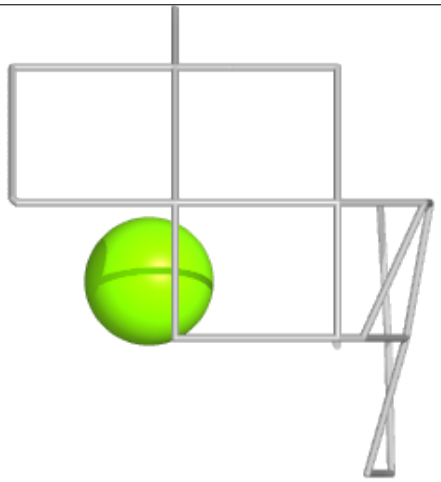


Electron density around MG B 1002:

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

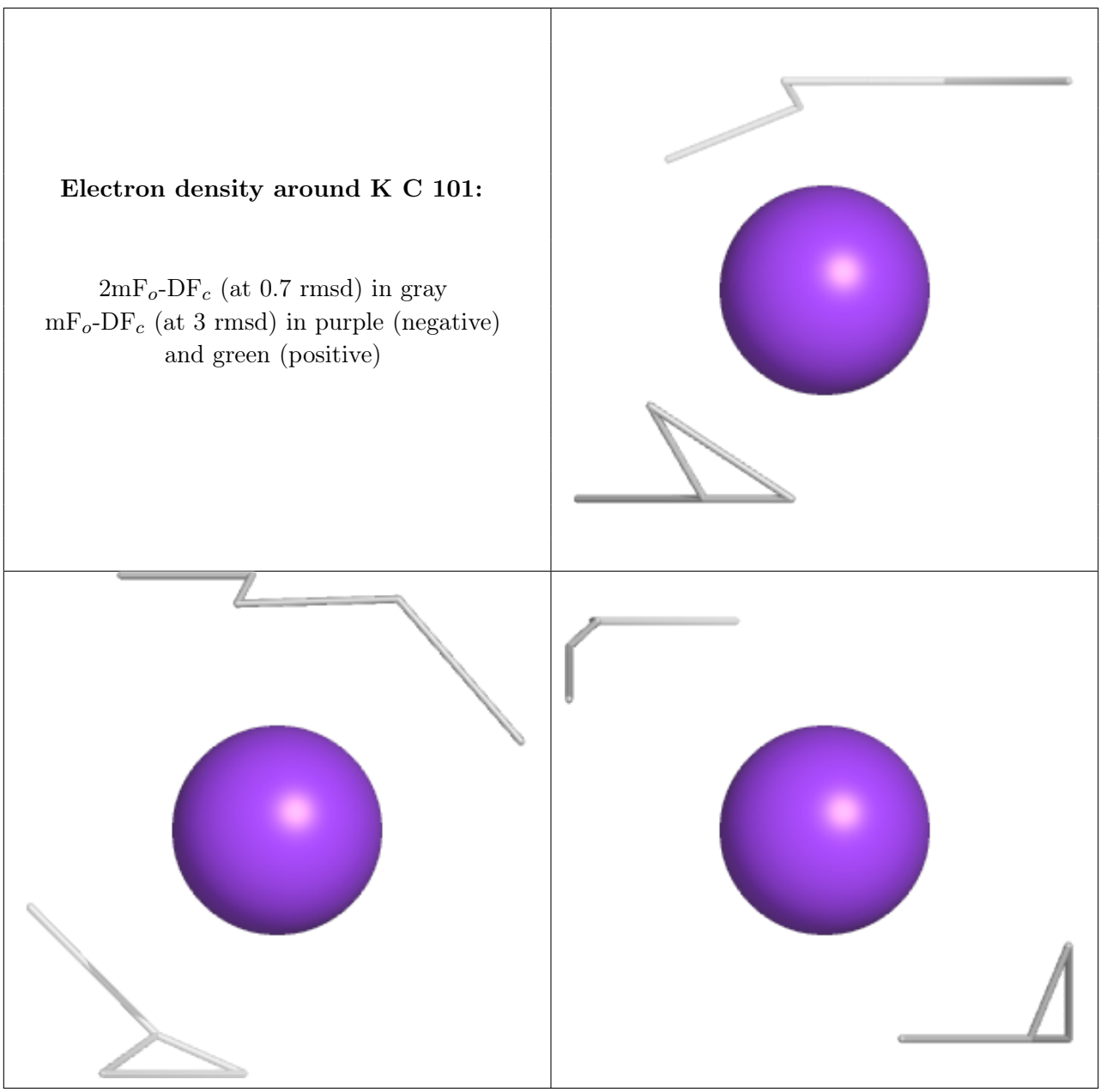






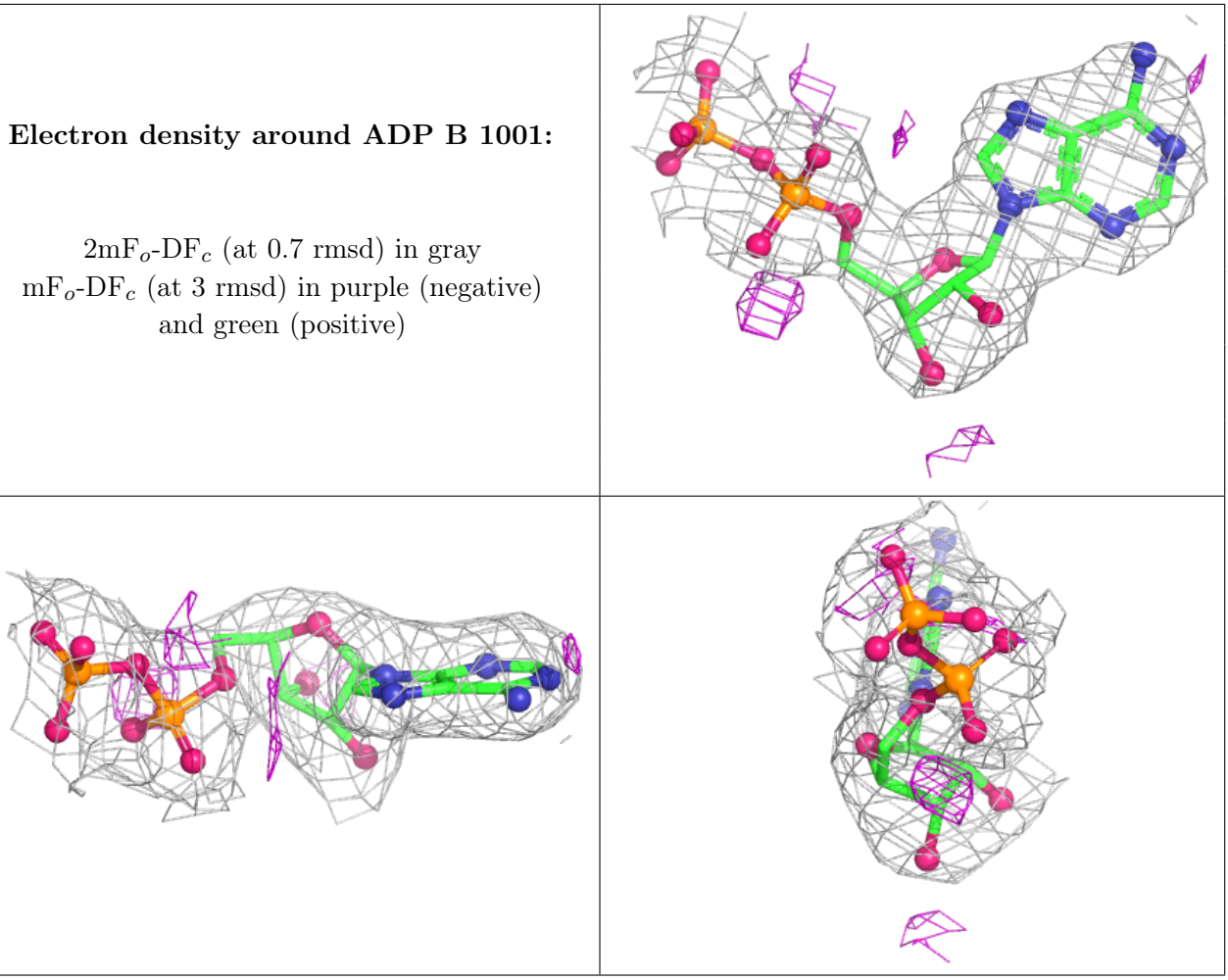
Electron density around K C 101:

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



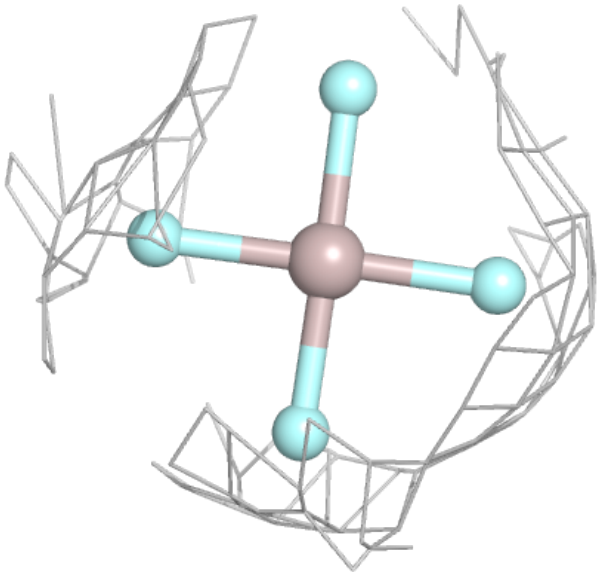
Electron density around ADP B 1001:

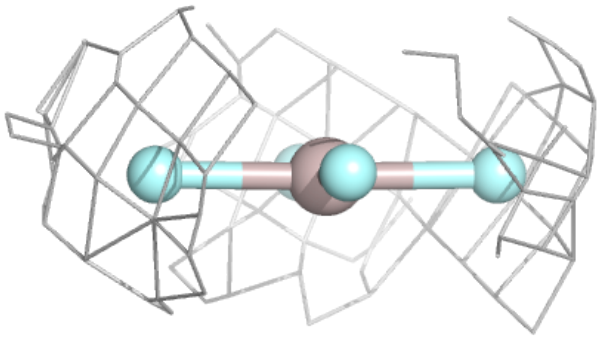
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

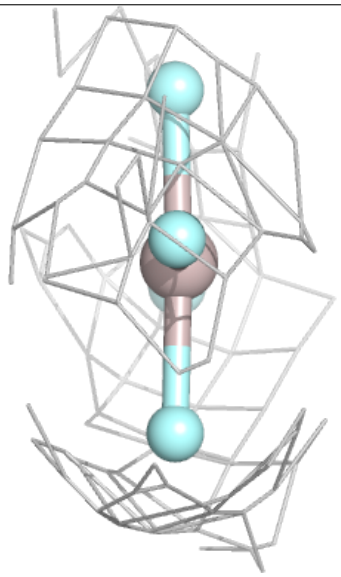


Electron density around ALF B 1003:

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

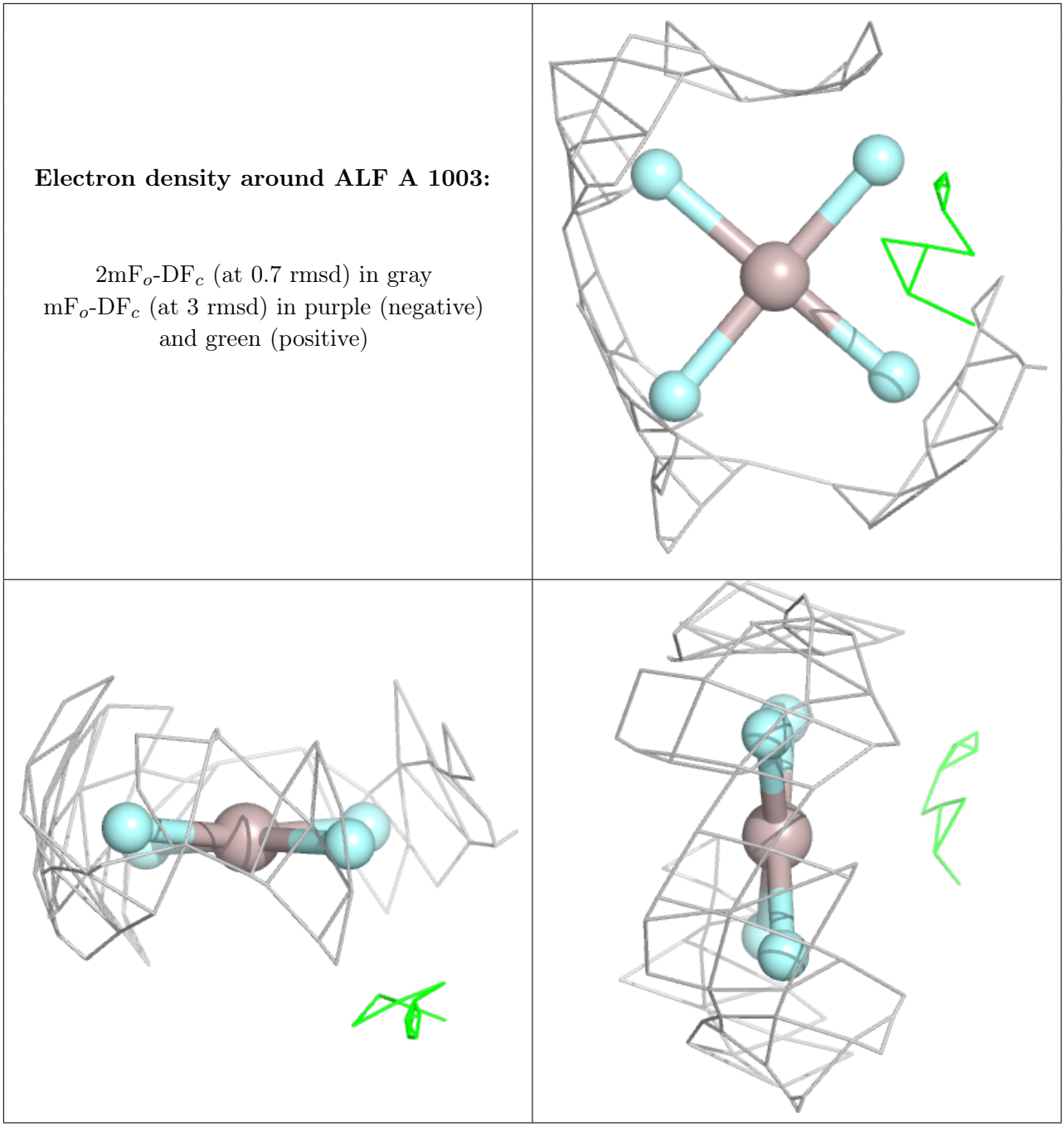






Electron density around ALF A 1003:

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



6.5 Other polymers

There are no such residues in this entry.