Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 12:21 pm GMT

PDB ID	:	8CGY
Title	:	Trypanosoma brucei IMP dehydrogenase (ori) crystallized in High Five cells reveals native ligands ATP, GDP and phosphate. Diffraction data collection at 100 K in cellulo; XDS processing
Authors	:	Boger, J.; Schoenherr, R.; Lahey-Rudolph, J.M.; Harms, M.; Kaiser, J.; Nachtschatt, S.; Wobbe, M.; Duden, R.; Bourenkov, G.; Schneider, T.; Redecke, L.
Deposited on	:	2023-02-06
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

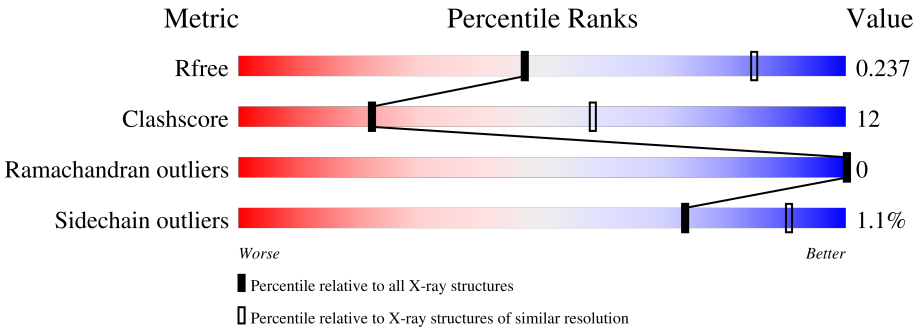
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Mol	Chain	Length	Quality of chain
1	A	512	70% 17% 13%
1	B	512	67% 20% 13%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6919 atoms, of which 72 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.

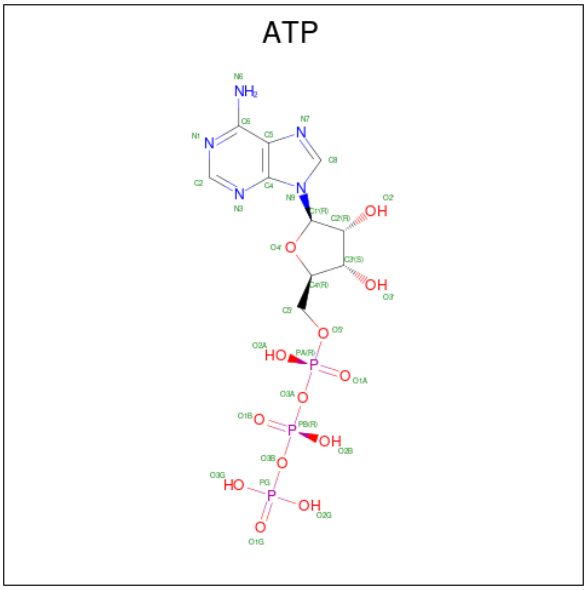
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3317	2070	587	639	21			
1	B	447	Total	C	N	O	S	0	0	0
			3338	2085	592	640	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	488	SER	THR	engineered mutation	UNP P50098
B	488	SER	THR	engineered mutation	UNP P50098

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	1
			86	20	24	10	26	6		

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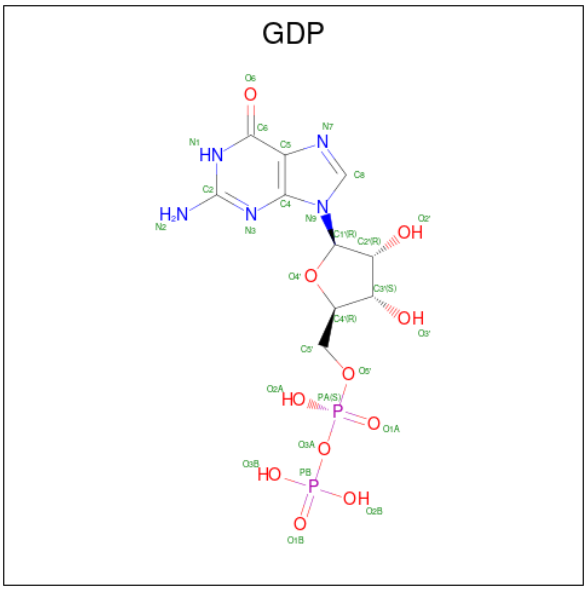
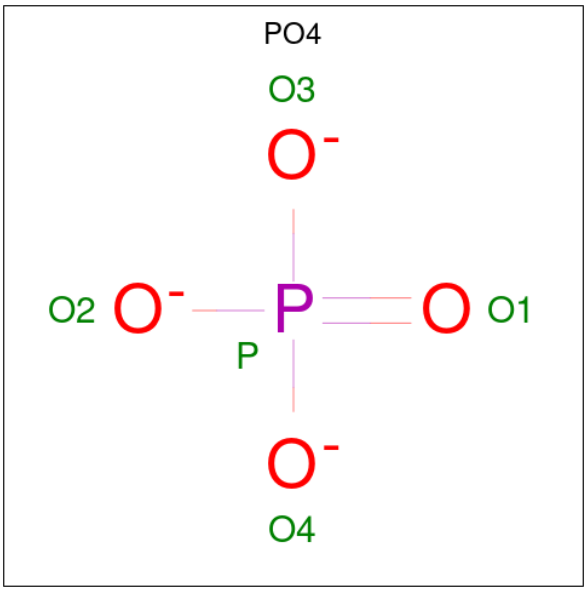
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	1
			86	20	24	10	26	6		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		
3	B	1	Total	C	H	N	O	P	0	0
			40	10	12	5	11	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

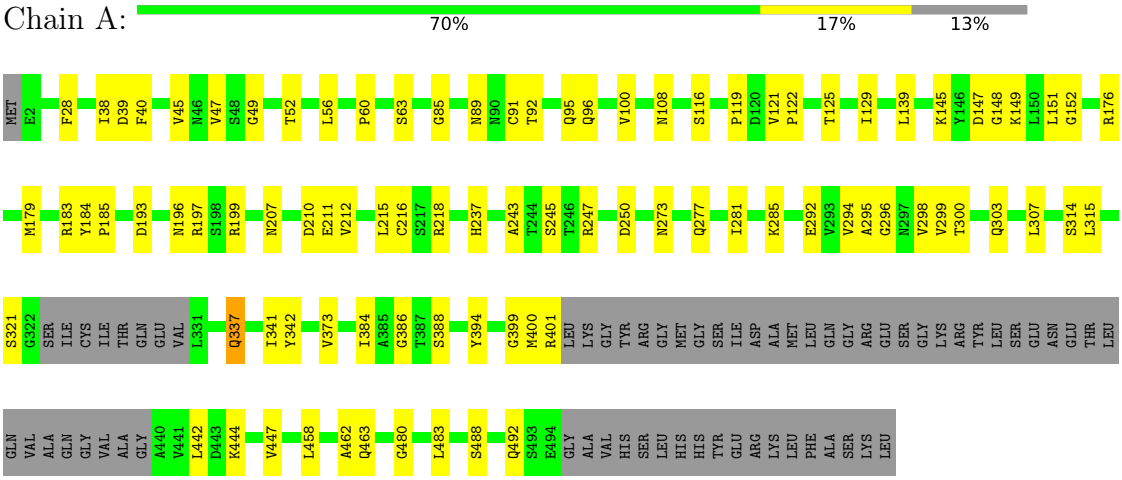
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0

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. 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. 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.

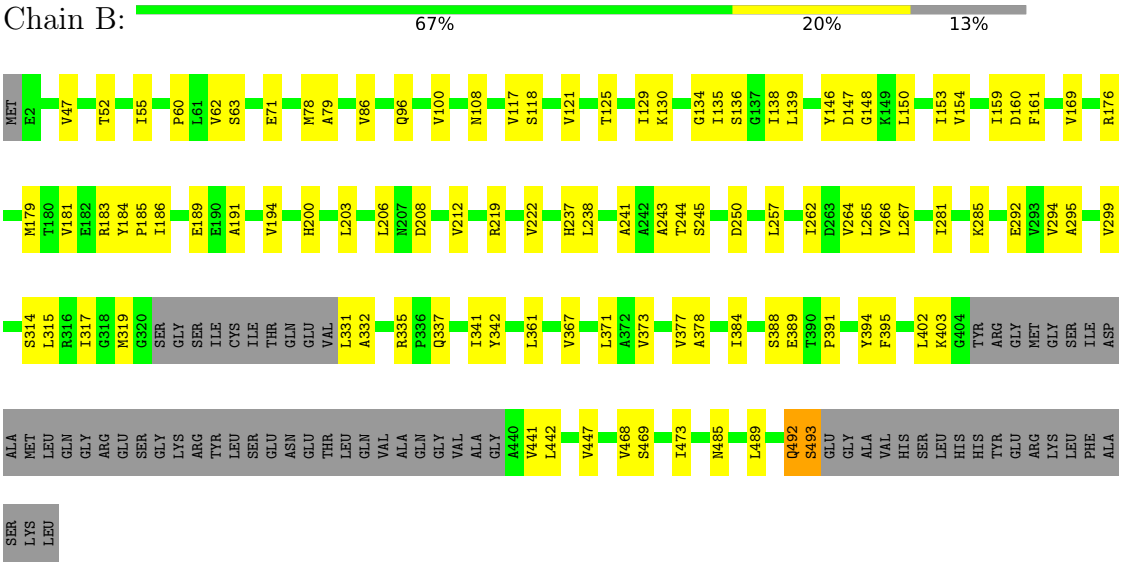
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain A:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	207.10Å 207.10Å 92.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.62 – 3.00 146.44 – 1.66	Depositor EDS
% Data completeness (in resolution range)	99.9 (92.62-3.00) 21.6 (146.44-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.192 , 0.237 0.194 , 0.237	Depositor DCC
R_{free} test set	2000 reflections (3.92%)	wwPDB-VP
Wilson B-factor (Å^2)	6.3	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	6919	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: PO4, GDP, 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	0.28	0/3362	0.54	0/4554
1	B	0.28	0/3383	0.54	0/4577
All	All	0.28	0/6745	0.54	0/9131

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3317	0	3276	69	0
1	B	3338	0	3324	89	0
2	A	62	24	24	0	0
2	B	62	24	24	1	0
3	A	28	12	10	2	0
3	B	28	12	11	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	2	0	0	0	0
All	All	6847	72	6669	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 12.

All (159) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:602:GDP:C4'	3:A:602:GDP:O4'	1.70	1.21
3:B:602:GDP:C4'	3:B:602:GDP:O4'	1.70	1.12
1:A:148:GLY:HA2	1:A:212:VAL:H	1.12	1.04
1:B:331:LEU:HG	1:B:332:ALA:H	1.38	0.88
1:B:47:VAL:HG23	1:B:60:PRO:HD3	1.56	0.87
1:A:148:GLY:HA3	1:A:211:GLU:HB3	1.63	0.80
1:A:321:SER:HB3	1:A:337:GLN:HG2	1.61	0.80
1:A:121:VAL:HG22	1:A:122:PRO:HD2	1.67	0.77
1:A:148:GLY:HA2	1:A:212:VAL:N	1.96	0.75
1:B:130:LYS:HD2	1:B:136:SER:HB2	1.69	0.74
1:A:342:TYR:HB2	1:A:373:VAL:HG13	1.72	0.72
1:A:176:ARG:HA	1:A:179:MET:CE	2.20	0.72
1:A:108:ASN:HB3	1:A:237:HIS:CE1	2.26	0.71
1:B:150:LEU:HD22	1:B:206:LEU:HD21	1.73	0.69
1:A:176:ARG:HA	1:A:179:MET:HE2	1.74	0.69
1:A:122:PRO:HG2	1:A:125:THR:HG23	1.75	0.68
1:A:152:GLY:HA2	1:A:179:MET:HE1	1.75	0.68
1:B:183:ARG:O	1:B:186:ILE:HG23	1.92	0.68
1:B:299:VAL:HG21	1:B:319:MET:HB3	1.76	0.67
1:A:245:SER:HB2	1:A:250:ASP:OD2	1.95	0.67
1:B:136:SER:O	1:B:136:SER:OG	2.12	0.66
1:A:298:VAL:HG13	1:A:303:GLN:HB2	1.78	0.66
1:B:117:VAL:HG13	1:B:121:VAL:HG21	1.76	0.65
1:B:342:TYR:HB2	1:B:373:VAL:CG1	2.27	0.64
1:A:121:VAL:CG2	1:A:122:PRO:HD2	2.29	0.63
1:B:138:ILE:H	1:B:138:ILE:HD12	1.64	0.63
1:A:295:ALA:HB1	1:A:307:LEU:HD13	1.81	0.63
1:B:184:TYR:HB3	1:B:185:PRO:HD3	1.81	0.62
1:B:63:SER:HB3	1:B:78:MET:HE2	1.81	0.62
1:A:294:VAL:HG22	1:A:314:SER:HB3	1.80	0.62
1:A:277:GLN:OE1	1:A:296:GLY:N	2.28	0.61
1:B:492:GLN:HG2	1:B:493:SER:N	2.15	0.61
1:B:62:VAL:HG23	1:B:377:VAL:HG11	1.83	0.61
1:B:299:VAL:CG1	1:B:335:ARG:HB3	2.30	0.61
1:A:52:THR:OG1	1:A:292:GLU:OE1	2.07	0.60
1:A:184:TYR:HB3	1:A:185:PRO:HD3	1.84	0.60
1:A:152:GLY:HA2	1:A:179:MET:CE	2.31	0.60
1:A:273:ASN:HB2	1:A:303:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG11	1:A:458:LEU:HD12	1.84	0.59
1:A:399:GLY:O	1:A:400:MET:HG3	2.03	0.58
1:B:62:VAL:HG23	1:B:377:VAL:CG1	2.34	0.58
1:B:337:GLN:HA	1:B:337:GLN:OE1	2.04	0.57
1:A:89:ASN:HB3	1:A:243:ALA:O	2.04	0.57
1:A:149:LYS:H	1:A:211:GLU:HA	1.68	0.57
1:B:146:TYR:O	1:B:212:VAL:HG13	2.05	0.57
1:A:92:THR:OG1	1:A:95:GLN:HG3	2.05	0.56
1:B:148:GLY:O	1:B:212:VAL:HG12	2.05	0.56
1:A:47:VAL:HG12	1:A:47:VAL:O	2.06	0.56
1:B:294:VAL:HG22	1:B:314:SER:HB3	1.88	0.56
1:A:96:GLN:O	1:A:100:VAL:HG23	2.06	0.56
1:B:469:SER:O	1:B:473:ILE:HG13	2.06	0.56
1:A:342:TYR:HB2	1:A:373:VAL:CG1	2.35	0.55
1:B:108:ASN:HB3	1:B:237:HIS:ND1	2.21	0.55
1:B:245:SER:HB2	1:B:250:ASP:OD2	2.05	0.55
1:B:47:VAL:HG23	1:B:60:PRO:CD	2.34	0.55
1:B:367:VAL:O	1:B:371:LEU:HG	2.08	0.54
1:B:186:ILE:HD12	1:B:191:ALA:HB2	1.89	0.54
1:A:321:SER:CB	1:A:337:GLN:HG2	2.36	0.53
1:B:96:GLN:O	1:B:100:VAL:HG23	2.07	0.53
1:B:468:VAL:O	1:B:468:VAL:HG12	2.08	0.53
1:A:247:ARG:HG2	1:A:250:ASP:OD2	2.08	0.53
1:B:299:VAL:HG11	1:B:335:ARG:CB	2.38	0.53
1:B:299:VAL:HG11	1:B:335:ARG:HB3	1.90	0.53
1:B:373:VAL:HG12	1:B:373:VAL:O	2.09	0.53
1:A:196:ASN:HA	1:A:218:ARG:NH2	2.24	0.52
1:A:298:VAL:HG13	1:A:303:GLN:CB	2.39	0.52
1:A:386:GLY:HA3	1:A:442:LEU:O	2.10	0.52
1:B:52:THR:OG1	1:B:292:GLU:OE1	2.18	0.52
1:B:138:ILE:HD12	1:B:138:ILE:N	2.22	0.52
1:A:176:ARG:HA	1:A:179:MET:HE3	1.90	0.51
1:B:153:ILE:HG13	1:B:179:MET:SD	2.50	0.51
1:A:394:TYR:CD1	1:A:401:ARG:HA	2.46	0.50
1:B:117:VAL:HG12	1:B:118:SER:O	2.12	0.50
1:A:193:ASP:OD1	1:A:197:ARG:NH1	2.44	0.50
1:B:299:VAL:CG1	1:B:335:ARG:HD2	2.41	0.50
1:B:159:ILE:HG22	1:B:159:ILE:O	2.12	0.50
1:B:395:PHE:CE1	1:B:402:LEU:HB2	2.46	0.50
1:A:488:SER:O	1:A:492:GLN:HG3	2.12	0.50
1:B:63:SER:HB3	1:B:78:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:VAL:HG12	1:B:118:SER:N	2.27	0.49
1:B:317:ILE:HG21	1:B:341:ILE:HA	1.94	0.49
1:A:218:ARG:NH1	1:B:160:ASP:OD2	2.38	0.49
1:B:299:VAL:HG13	1:B:335:ARG:HB3	1.95	0.49
1:A:299:VAL:HG23	1:A:300:THR:HG23	1.94	0.49
1:B:361:LEU:CD1	1:B:378:ALA:HB1	2.43	0.49
1:B:200:HIS:HA	2:B:601[B]:ATP:O1A	2.13	0.48
1:A:295:ALA:HB3	1:A:315:LEU:HD23	1.95	0.48
1:B:62:VAL:CG2	1:B:377:VAL:HG11	2.42	0.48
1:B:79:ALA:HB3	1:B:238:LEU:HD13	1.95	0.48
1:B:154:VAL:HG21	1:B:169:VAL:CG2	2.44	0.48
1:A:384:ILE:HG23	1:A:447:VAL:HG23	1.96	0.47
1:B:441:VAL:HG22	1:B:442:LEU:N	2.29	0.47
1:B:135:ILE:HG23	3:B:602:GDP:C6	2.49	0.47
1:B:299:VAL:CG1	1:B:335:ARG:CB	2.92	0.47
1:A:45:VAL:HG11	1:A:462:ALA:HB3	1.96	0.47
1:A:125:THR:O	1:A:129:ILE:HG13	2.14	0.47
1:B:154:VAL:HG21	1:B:169:VAL:HG22	1.97	0.47
1:A:337:GLN:O	1:A:341:ILE:HG13	2.14	0.47
1:B:299:VAL:HG21	1:B:319:MET:CB	2.43	0.47
1:B:71:GLU:HG3	1:B:391:PRO:HG3	1.97	0.47
1:B:147:ASP:OD1	1:B:147:ASP:N	2.48	0.47
1:B:117:VAL:HG23	1:B:138:ILE:CG2	2.45	0.46
1:B:219:ARG:HA	1:B:222:VAL:HG22	1.97	0.46
1:B:244:THR:CG2	1:B:265:LEU:HD11	2.45	0.46
3:A:602:GDP:O4'	3:A:602:GDP:C5'	2.54	0.46
1:A:38:ILE:HD13	1:A:463:GLN:HG2	1.97	0.46
1:B:189:GLU:N	1:B:189:GLU:OE1	2.48	0.46
1:B:384:ILE:HG22	1:B:384:ILE:O	2.16	0.46
1:B:130:LYS:O	1:B:134:GLY:HA2	2.15	0.45
1:B:257:LEU:HB3	1:B:262:ILE:HG21	1.98	0.45
1:A:116:SER:HA	1:A:139:LEU:O	2.17	0.45
1:B:394:TYR:CZ	1:B:403:LYS:HE2	2.52	0.45
1:A:39:ASP:OD1	1:A:40:PHE:HD1	1.99	0.45
1:A:281:ILE:O	1:A:285:LYS:HG2	2.17	0.45
1:B:373:VAL:CG1	1:B:373:VAL:O	2.64	0.45
1:B:86:VAL:HA	1:B:241:ALA:O	2.17	0.45
1:B:136:SER:HB3	1:B:219:ARG:HH12	1.82	0.45
1:B:208:ASP:N	1:B:208:ASP:OD1	2.49	0.45
1:B:331:LEU:HG	1:B:332:ALA:N	2.17	0.45
1:A:480:GLY:O	1:A:483:LEU:HD21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PRO:HG3	1:A:151:LEU:HD12	1.98	0.44
1:A:388:SER:HA	1:A:394:TYR:OH	2.17	0.44
1:B:117:VAL:N	1:B:139:LEU:O	2.45	0.44
1:A:273:ASN:CB	1:A:303:GLN:HG2	2.45	0.44
1:B:489:LEU:HD23	1:B:489:LEU:HA	1.82	0.44
1:A:47:VAL:HG12	1:A:60:PRO:CD	2.47	0.44
1:B:267:LEU:HD11	1:B:281:ILE:HG12	2.01	0.43
1:B:388:SER:HA	1:B:394:TYR:OH	2.18	0.43
1:B:191:ALA:O	1:B:194:VAL:HG22	2.18	0.43
1:B:194:VAL:HG23	1:B:203:LEU:HD22	2.00	0.43
1:B:244:THR:HG21	1:B:265:LEU:HD11	2.00	0.43
1:A:199:ARG:HH21	1:B:161:PHE:HZ	1.65	0.43
1:B:395:PHE:CZ	1:B:402:LEU:HB2	2.54	0.43
1:A:215:LEU:HD12	1:A:216:CYS:H	1.84	0.43
1:B:55:ILE:HD12	1:B:264:VAL:CG2	2.49	0.43
1:A:108:ASN:HB3	1:A:237:HIS:ND1	2.33	0.43
1:A:145:LYS:C	1:A:147:ASP:H	2.22	0.43
1:B:181:VAL:HA	1:B:203:LEU:HD12	1.99	0.43
1:A:49:GLY:O	1:A:56:LEU:HD12	2.19	0.42
1:B:125:THR:O	1:B:129:ILE:HG12	2.18	0.42
1:B:295:ALA:HB3	1:B:315:LEU:HD23	2.01	0.42
1:B:117:VAL:CG1	1:B:121:VAL:HG21	2.48	0.42
1:A:47:VAL:HG12	1:A:60:PRO:HD3	2.01	0.42
1:A:386:GLY:H	1:A:444:LYS:HD2	1.84	0.42
1:B:384:ILE:HD12	1:B:447:VAL:HG23	2.02	0.42
1:A:91:CYS:SG	1:A:96:GLN:HB2	2.60	0.42
1:B:243:ALA:HA	1:B:266:VAL:O	2.20	0.42
1:B:402:LEU:HD23	1:B:442:LEU:HA	2.02	0.42
1:A:47:VAL:HG12	1:A:60:PRO:HG3	2.02	0.41
1:A:384:ILE:HG23	1:A:384:ILE:HD12	1.88	0.41
1:A:149:LYS:N	1:A:211:GLU:HA	2.34	0.41
1:B:153:ILE:HG13	1:B:179:MET:CE	2.50	0.41
1:A:47:VAL:O	1:A:47:VAL:CG1	2.69	0.41
1:A:28:PHE:HZ	1:A:341:ILE:HD12	1.85	0.40
1:A:63:SER:OG	1:A:85:GLY:HA2	2.22	0.40
1:A:295:ALA:O	1:A:296:GLY:O	2.38	0.40
1:B:389:GLU:OE1	1:B:389:GLU:N	2.54	0.40
1:B:285:LYS:HA	1:B:285:LYS:HD2	1.94	0.40
1:B:299:VAL:HG11	1:B:335:ARG:HB2	2.03	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	441/512 (86%)	417 (95%)	24 (5%)	0	100	100
1	B	441/512 (86%)	423 (96%)	18 (4%)	0	100	100
All	All	882/1024 (86%)	840 (95%)	42 (5%)	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	351/423 (83%)	347 (99%)	4 (1%)	73	90
1	B	355/423 (84%)	351 (99%)	4 (1%)	73	90
All	All	706/846 (84%)	698 (99%)	8 (1%)	73	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	ARG
1	A	207	ASN
1	A	210	ASP
1	A	337	GLN
1	B	176	ARG
1	B	485	ASN
1	B	492	GLN
1	B	493	SER

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ATP	A	601[B]	-	26,33,33	4.80	7 (26%)	31,52,52	1.68	4 (12%)
3	GDP	B	602	-	24,30,30	4.07	13 (54%)	30,47,47	1.49	5 (16%)
4	PO4	A	603	-	4,4,4	0.93	0	6,6,6	0.45	0
2	ATP	B	601[B]	-	26,33,33	4.76	7 (26%)	31,52,52	1.44	5 (16%)
2	ATP	B	601[A]	-	26,33,33	4.76	6 (23%)	31,52,52	1.43	5 (16%)
2	ATP	A	601[A]	-	26,33,33	4.72	7 (26%)	31,52,52	1.58	6 (19%)
4	PO4	B	603	-	4,4,4	0.92	0	6,6,6	0.52	0
3	GDP	A	602	-	24,30,30	4.24	13 (54%)	30,47,47	1.50	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	601[B]	-	-	4/18/38/38	0/3/3/3
3	GDP	B	602	-	-	6/12/32/32	0/3/3/3
2	ATP	B	601[B]	-	-	4/18/38/38	0/3/3/3
2	ATP	B	601[A]	-	-	2/18/38/38	0/3/3/3
2	ATP	A	601[A]	-	-	5/18/38/38	0/3/3/3
3	GDP	A	602	-	-	4/12/32/32	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601[B]	ATP	O4'-C1'	15.88	1.63	1.41
2	B	601[B]	ATP	O4'-C1'	15.77	1.63	1.41
2	B	601[A]	ATP	O4'-C1'	15.60	1.62	1.41
2	A	601[A]	ATP	O4'-C1'	15.44	1.62	1.41
2	B	601[A]	ATP	C2'-C1'	-14.53	1.31	1.53
2	B	601[B]	ATP	C2'-C1'	-14.42	1.31	1.53
2	A	601[B]	ATP	C2'-C1'	-14.39	1.31	1.53
2	A	601[A]	ATP	C2'-C1'	-14.18	1.32	1.53
3	A	602	GDP	O4'-C4'	11.33	1.70	1.45
3	B	602	GDP	O4'-C4'	11.19	1.70	1.45
3	A	602	GDP	C3'-C4'	-9.08	1.29	1.53
2	B	601[A]	ATP	O4'-C4'	-8.77	1.25	1.45
2	A	601[A]	ATP	O4'-C4'	-8.68	1.25	1.45
3	B	602	GDP	C3'-C4'	-8.57	1.31	1.53
2	B	601[B]	ATP	O4'-C4'	-8.49	1.26	1.45
2	A	601[B]	ATP	O4'-C4'	-8.49	1.26	1.45
3	A	602	GDP	O4'-C1'	-7.28	1.30	1.41
3	B	602	GDP	O4'-C1'	-6.24	1.32	1.41
2	A	601[B]	ATP	O2'-C2'	5.89	1.56	1.43
2	A	601[A]	ATP	O2'-C2'	5.62	1.56	1.43
3	A	602	GDP	C2-N3	5.43	1.46	1.33
2	B	601[A]	ATP	O2'-C2'	5.32	1.55	1.43
3	B	602	GDP	C2-N3	5.28	1.46	1.33
2	B	601[B]	ATP	O2'-C2'	5.15	1.55	1.43
3	A	602	GDP	C2-N2	4.79	1.45	1.34
3	A	602	GDP	O2'-C2'	-4.72	1.31	1.43
3	B	602	GDP	C4-N3	4.71	1.48	1.37
3	A	602	GDP	C4-N3	4.68	1.48	1.37
3	B	602	GDP	O2'-C2'	-4.68	1.32	1.43
3	B	602	GDP	C2-N2	4.53	1.45	1.34
3	A	602	GDP	C6-N1	4.51	1.44	1.37
3	B	602	GDP	C6-N1	4.26	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	GDP	C2'-C1'	3.41	1.58	1.53
2	A	601[B]	ATP	C6-N6	3.14	1.45	1.34
2	A	601[A]	ATP	C6-N6	3.13	1.45	1.34
2	B	601[B]	ATP	C6-N6	3.10	1.45	1.34
2	B	601[A]	ATP	C6-N6	3.04	1.45	1.34
3	A	602	GDP	C2-N1	3.03	1.45	1.37
3	B	602	GDP	C2'-C1'	2.95	1.58	1.53
3	B	602	GDP	C2-N1	2.70	1.44	1.37
3	A	602	GDP	O3'-C3'	2.67	1.49	1.43
3	B	602	GDP	C5-C6	2.64	1.52	1.47
3	B	602	GDP	O3'-C3'	2.61	1.49	1.43
2	A	601[B]	ATP	PA-O5'	2.23	1.68	1.59
3	A	602	GDP	O6-C6	-2.20	1.18	1.23
3	B	602	GDP	O6-C6	-2.14	1.18	1.23
2	B	601[B]	ATP	PB-O1B	2.12	1.58	1.50
2	A	601[B]	ATP	PB-O1B	2.11	1.58	1.50
2	A	601[A]	ATP	PA-O5'	2.10	1.67	1.59
2	A	601[A]	ATP	C3'-C4'	2.08	1.58	1.53
3	A	602	GDP	C5-C6	2.07	1.51	1.47
2	B	601[A]	ATP	PB-O1B	2.02	1.58	1.50
2	B	601[B]	ATP	PA-O5'	2.00	1.67	1.59

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601[A]	ATP	N3-C2-N1	-4.77	121.22	128.68
2	B	601[B]	ATP	N3-C2-N1	-4.77	121.22	128.68
2	B	601[A]	ATP	N3-C2-N1	-4.76	121.24	128.68
2	A	601[B]	ATP	PA-O3A-PB	-4.75	116.52	132.83
2	A	601[B]	ATP	N3-C2-N1	-4.71	121.32	128.68
3	B	602	GDP	C5-C6-N1	3.37	119.90	113.95
3	B	602	GDP	PA-O3A-PB	-3.22	121.77	132.83
3	A	602	GDP	C5-C6-N1	3.16	119.54	113.95
3	B	602	GDP	C8-N7-C5	3.07	108.84	102.99
2	A	601[A]	ATP	O4'-C1'-C2'	-3.01	102.52	106.93
3	B	602	GDP	C2-N1-C6	-2.90	119.75	125.10
3	A	602	GDP	C8-N7-C5	2.82	108.36	102.99
3	A	602	GDP	C2-N1-C6	-2.79	119.96	125.10
3	A	602	GDP	O6-C6-C5	-2.75	119.00	124.37
2	A	601[A]	ATP	PA-O3A-PB	-2.72	123.50	132.83
2	B	601[B]	ATP	O4'-C1'-C2'	-2.51	103.26	106.93
2	B	601[A]	ATP	PB-O3B-PG	-2.37	124.70	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	GDP	C2'-C3'-C4'	2.36	107.24	102.64
2	A	601[A]	ATP	O5'-C5'-C4'	2.31	116.95	108.99
2	A	601[B]	ATP	C3'-C2'-C1'	2.25	104.36	100.98
2	B	601[A]	ATP	C1'-N9-C4	-2.24	122.70	126.64
2	B	601[B]	ATP	PA-O3A-PB	-2.19	125.31	132.83
2	A	601[B]	ATP	PB-O3B-PG	-2.18	125.33	132.83
2	B	601[B]	ATP	C1'-N9-C4	-2.18	122.81	126.64
2	A	601[A]	ATP	PB-O3B-PG	-2.18	125.34	132.83
2	B	601[A]	ATP	O4'-C1'-C2'	-2.18	103.75	106.93
2	B	601[A]	ATP	PA-O3A-PB	-2.16	125.42	132.83
2	B	601[B]	ATP	PB-O3B-PG	-2.15	125.45	132.83
3	A	602	GDP	N2-C2-N1	2.09	121.16	116.71
2	A	601[A]	ATP	O3G-PG-O3B	2.06	111.53	104.64
3	B	602	GDP	C2'-C3'-C4'	2.03	106.58	102.64

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601[B]	ATP	O4'-C4'-C5'-O5'
2	B	601[B]	ATP	C3'-C4'-C5'-O5'
3	A	602	GDP	C5'-O5'-PA-O1A
3	B	602	GDP	C5'-O5'-PA-O3A
3	B	602	GDP	C5'-O5'-PA-O2A
3	B	602	GDP	C3'-C4'-C5'-O5'
3	B	602	GDP	O4'-C4'-C5'-O5'
3	B	602	GDP	C4'-C5'-O5'-PA
2	A	601[A]	ATP	C4'-C5'-O5'-PA
3	A	602	GDP	C4'-C5'-O5'-PA
2	B	601[A]	ATP	PB-O3B-PG-O1G
2	A	601[A]	ATP	PB-O3A-PA-O1A
2	A	601[B]	ATP	PA-O3A-PB-O3B
2	A	601[A]	ATP	PB-O3A-PA-O5'
2	A	601[B]	ATP	C4'-C5'-O5'-PA
2	B	601[A]	ATP	PG-O3B-PB-O1B
3	B	602	GDP	C5'-O5'-PA-O1A
2	A	601[B]	ATP	PG-O3B-PB-O2B
2	B	601[B]	ATP	PB-O3A-PA-O1A
2	A	601[A]	ATP	C5'-O5'-PA-O3A
3	A	602	GDP	C5'-O5'-PA-O3A
3	A	602	GDP	O4'-C4'-C5'-O5'
2	A	601[A]	ATP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	A	601[B]	ATP	PG-O3B-PB-O1B
2	B	601[B]	ATP	PB-O3A-PA-O2A

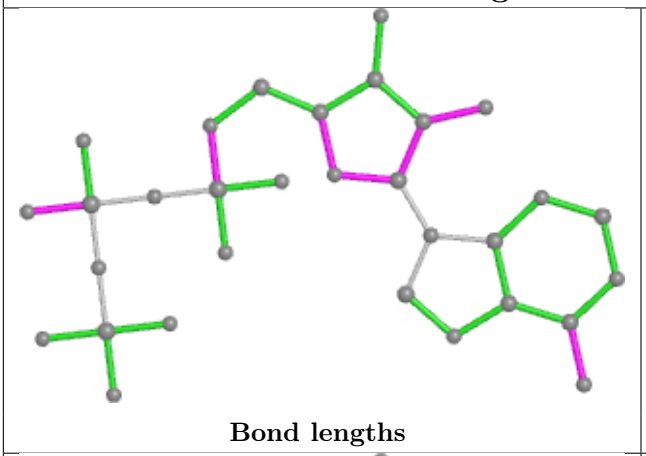
There are no ring outliers.

3 monomers are involved in 5 short contacts:

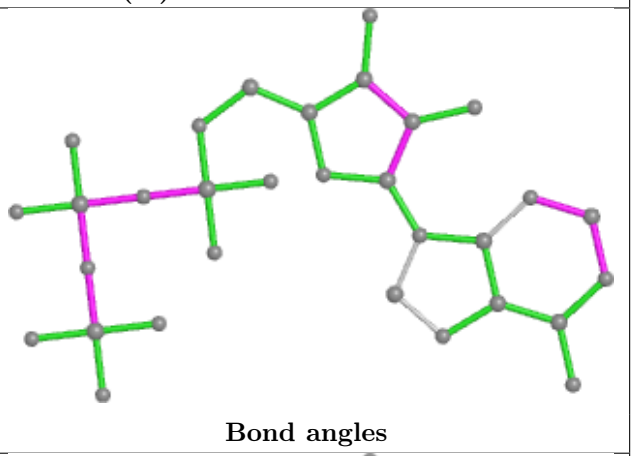
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GDP	2	0
2	B	601[B]	ATP	1	0
3	A	602	GDP	2	0

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.

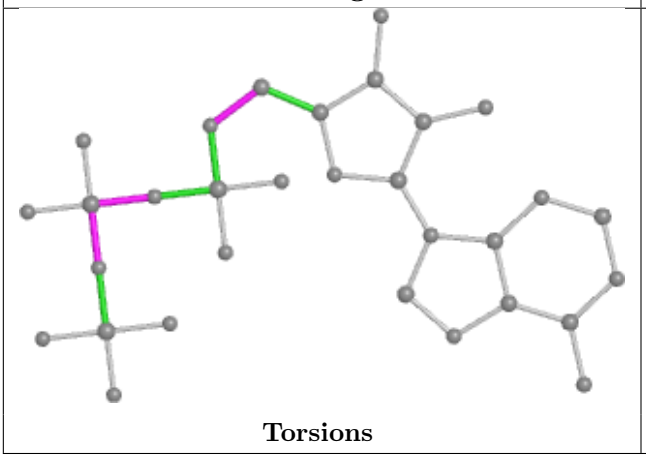
Ligand ATP A 601 (B)



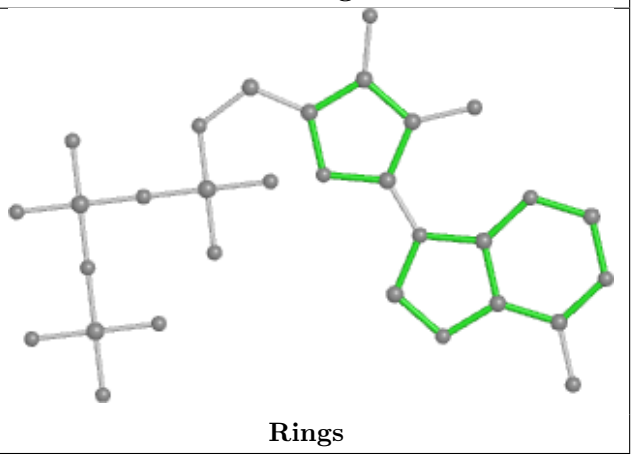
Bond lengths



Bond angles

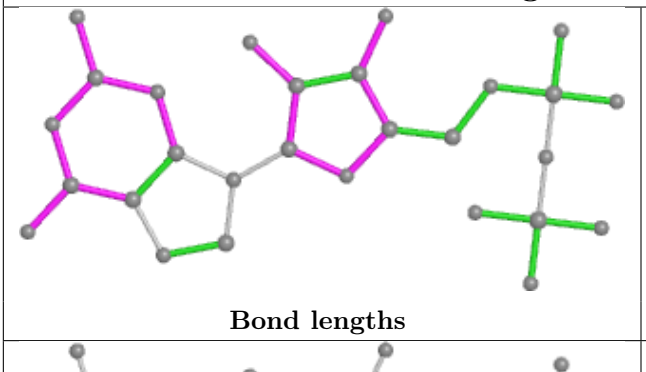


Torsions

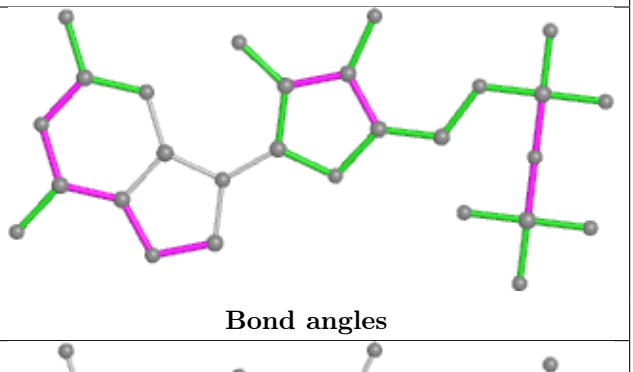


Rings

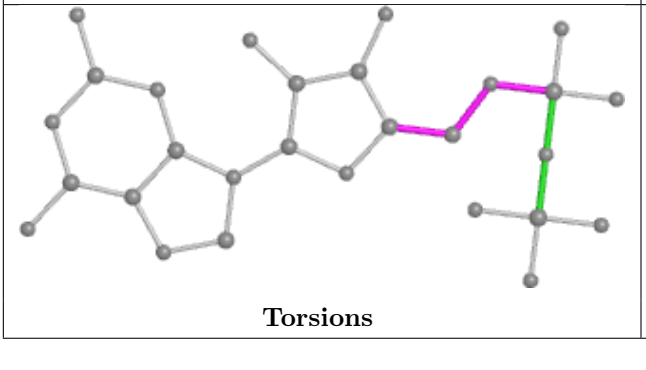
Ligand GDP B 602



Bond lengths



Bond angles



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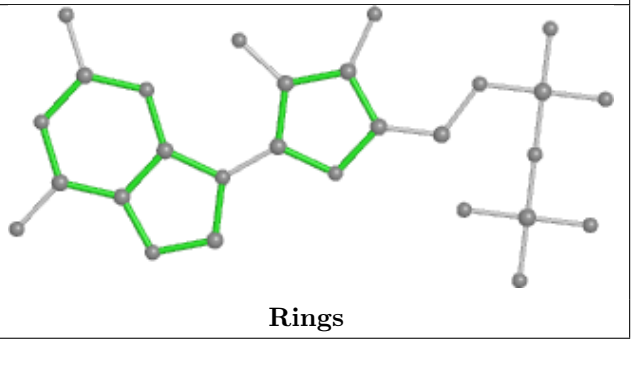
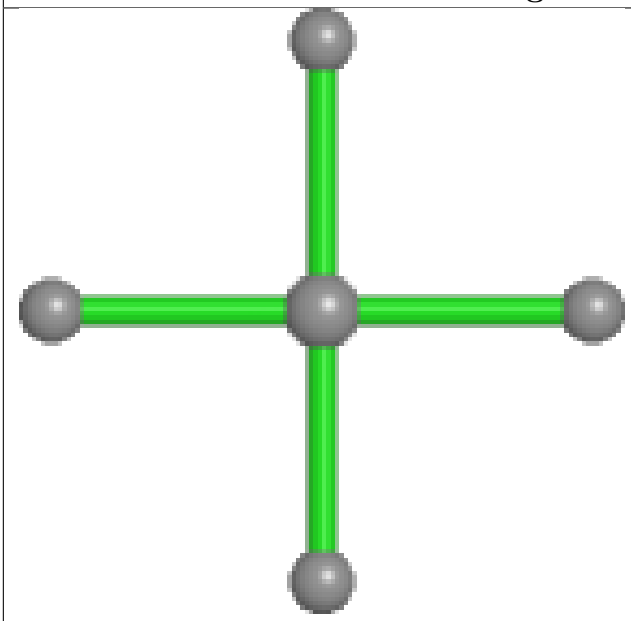
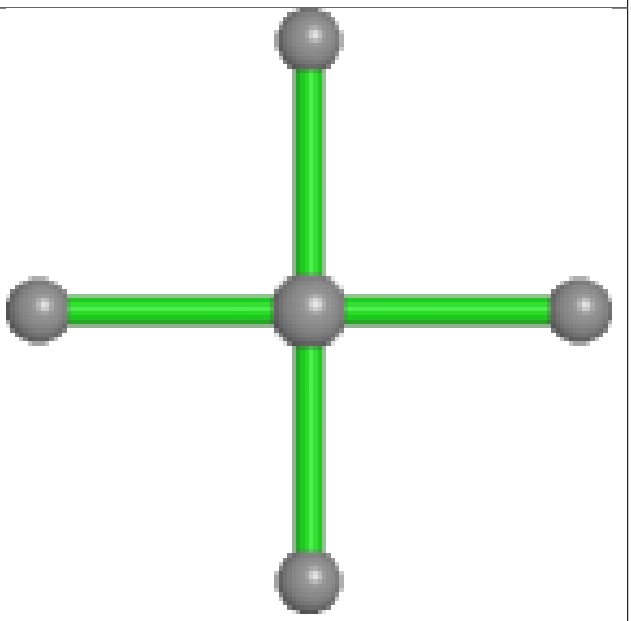


Rings

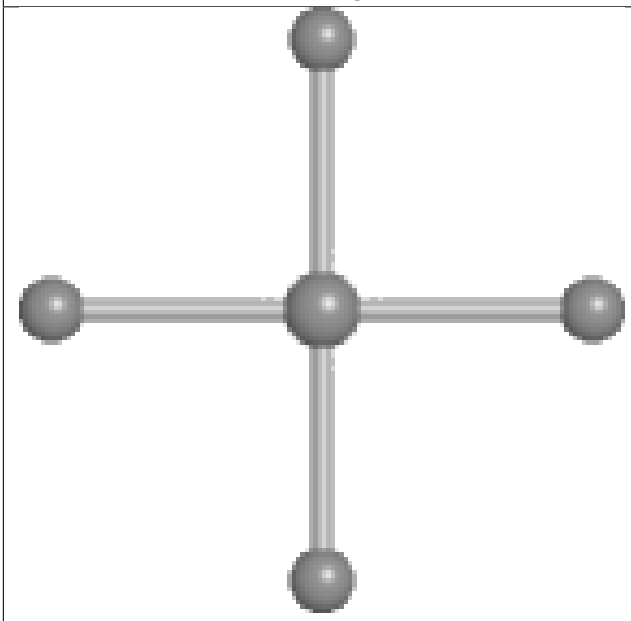
Ligand PO4 A 603



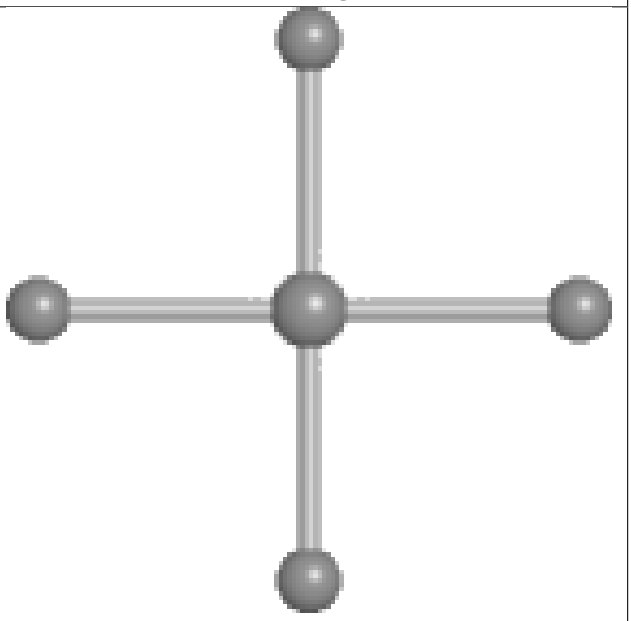
Bond lengths



Bond angles

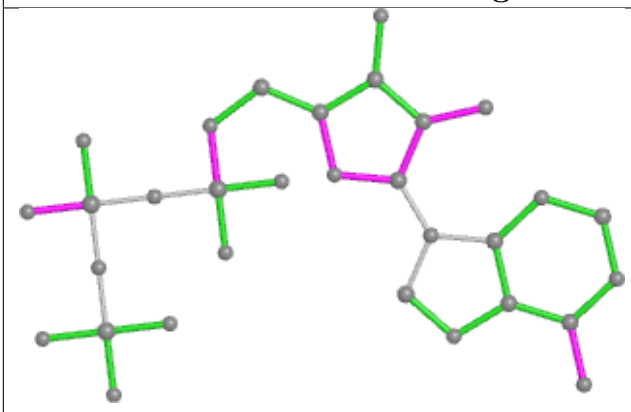


Torsions

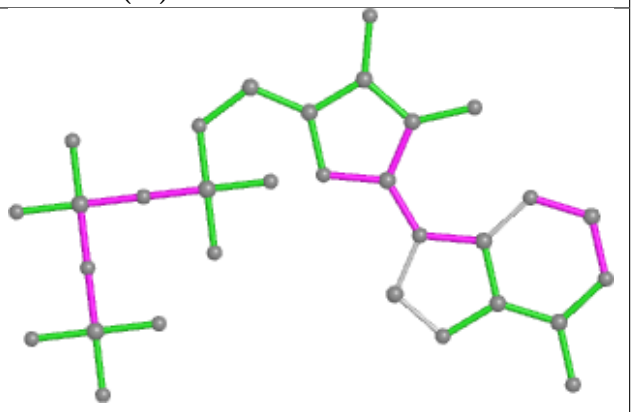


Rings

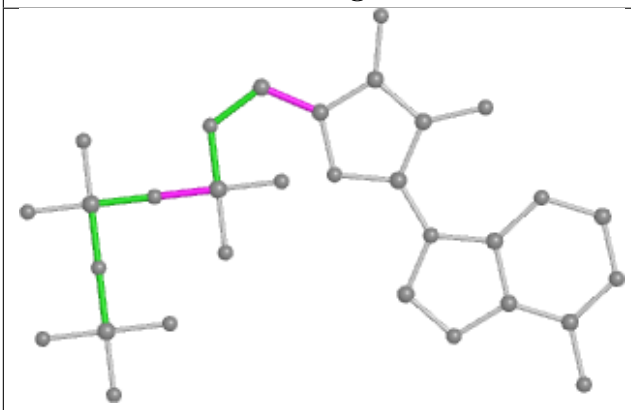
Ligand ATP B 601 (B)



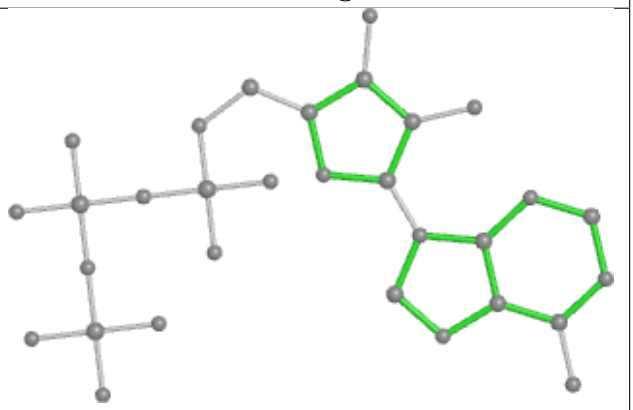
Bond lengths



Bond angles

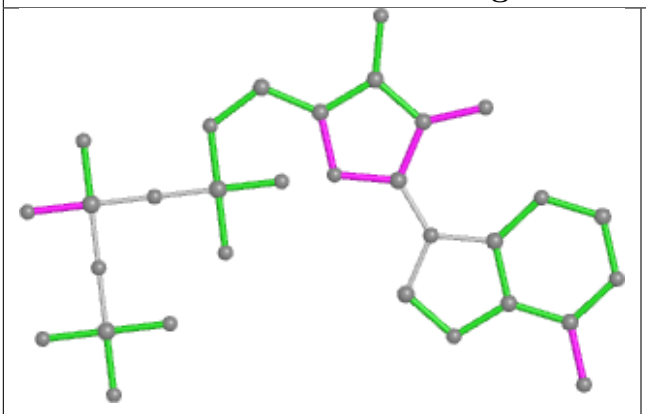


Torsions

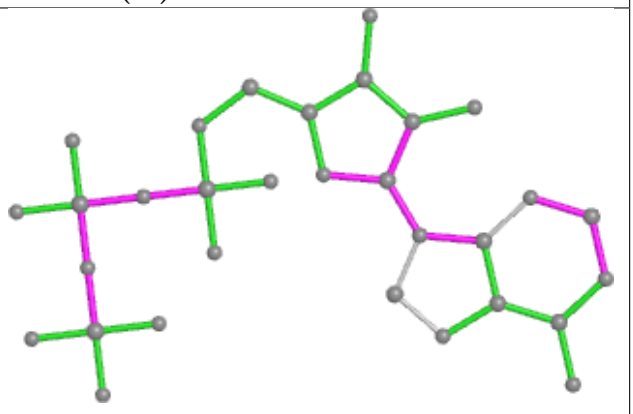


Rings

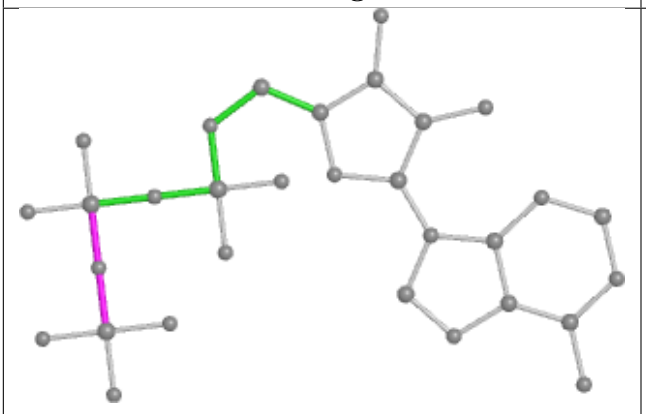
Ligand ATP B 601 (A)



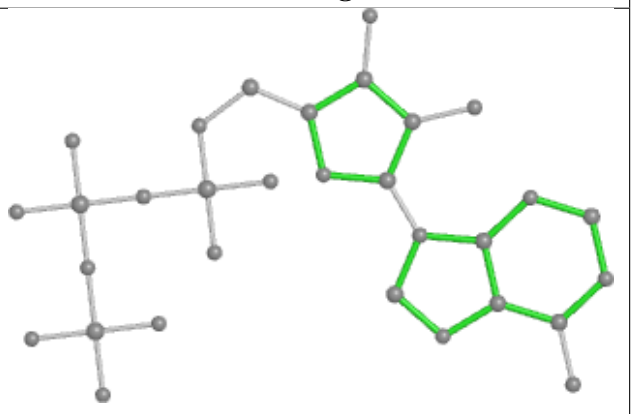
Bond lengths



Bond angles

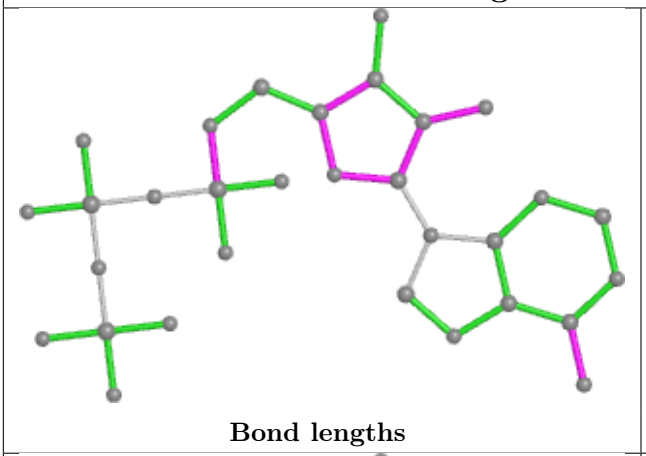


Torsions

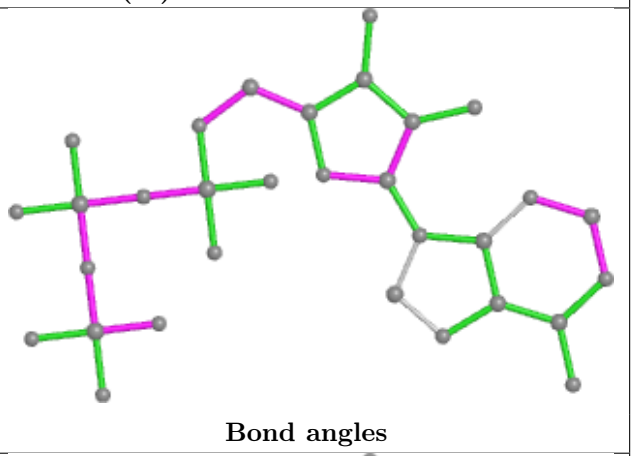


Rings

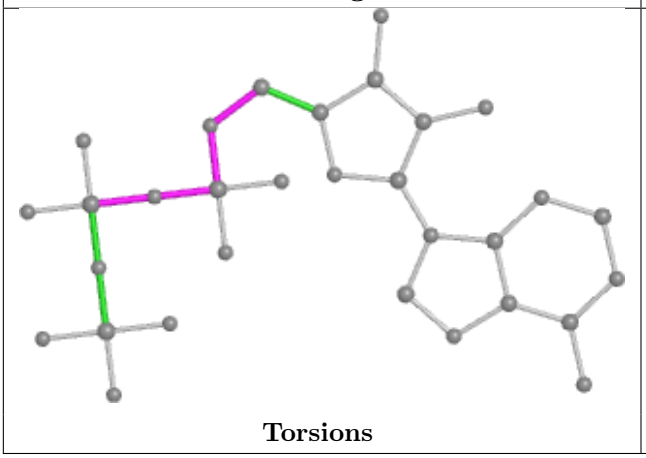
Ligand ATP A 601 (A)



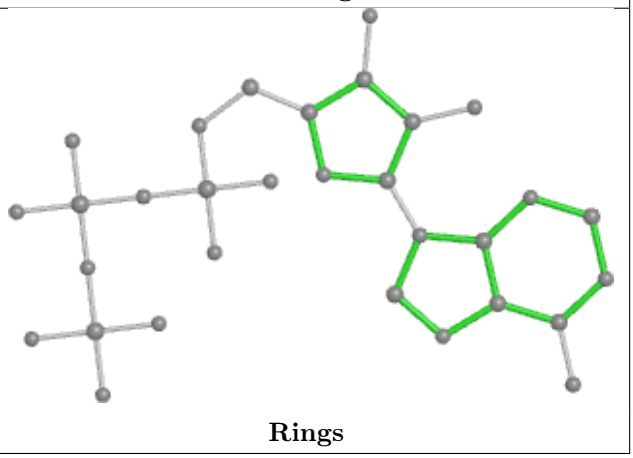
Bond lengths



Bond angles

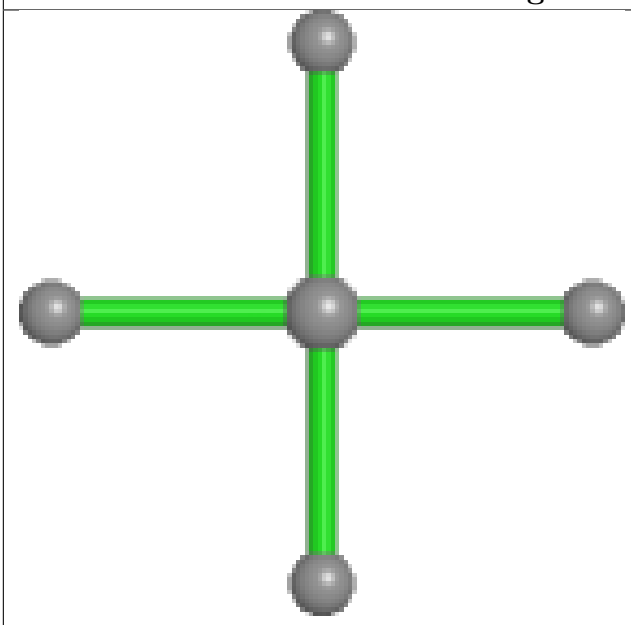


Torsions

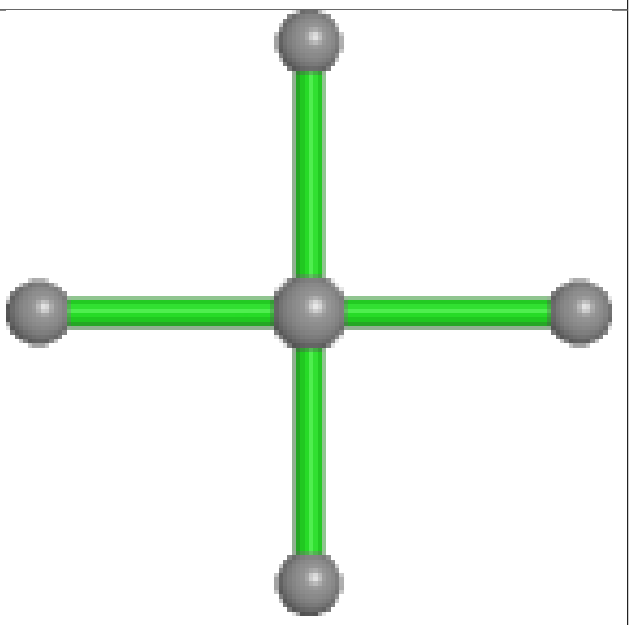


Rings

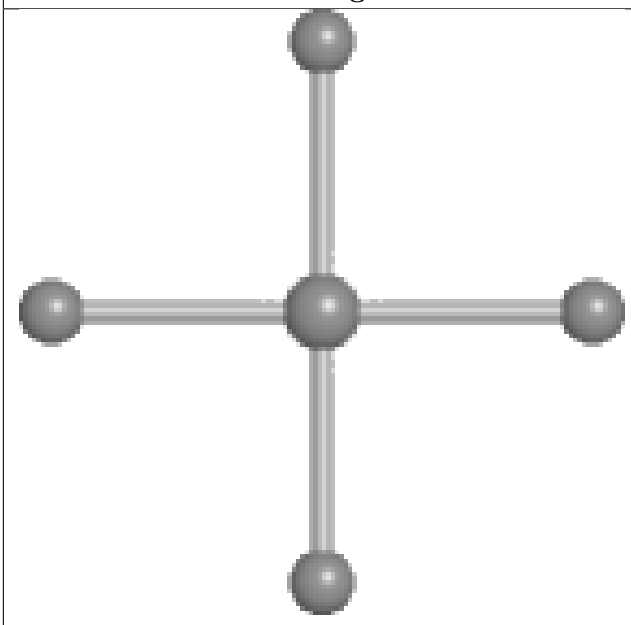
Ligand PO4 B 603



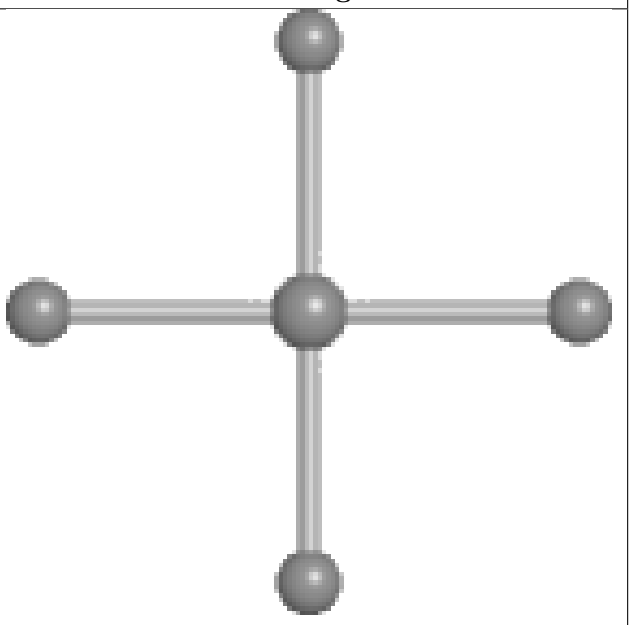
Bond lengths



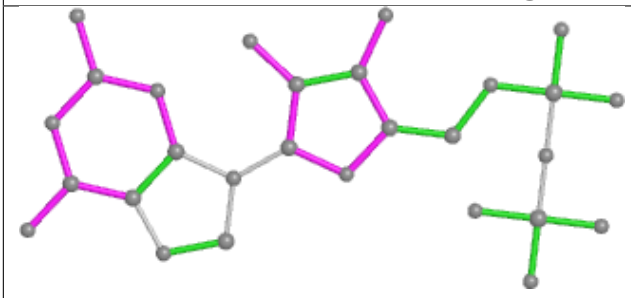
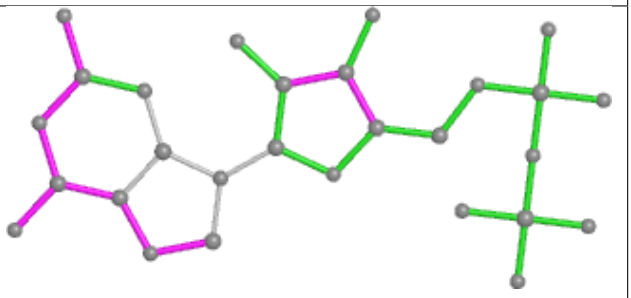
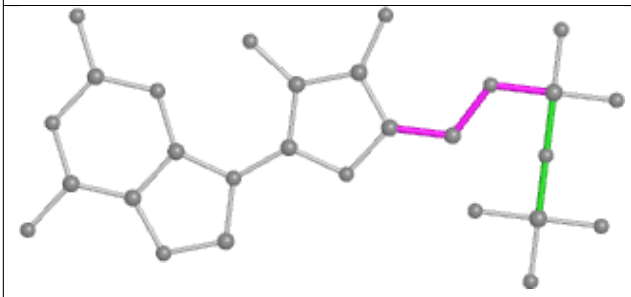
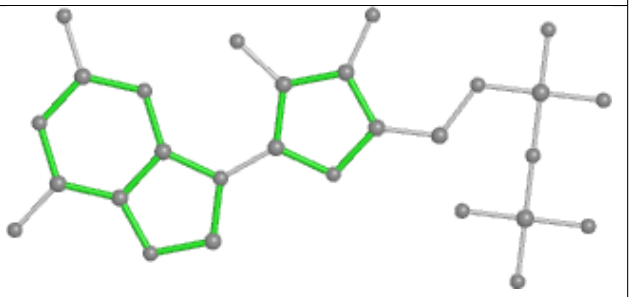
Bond angles



Torsions



Rings

Ligand GDP A 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

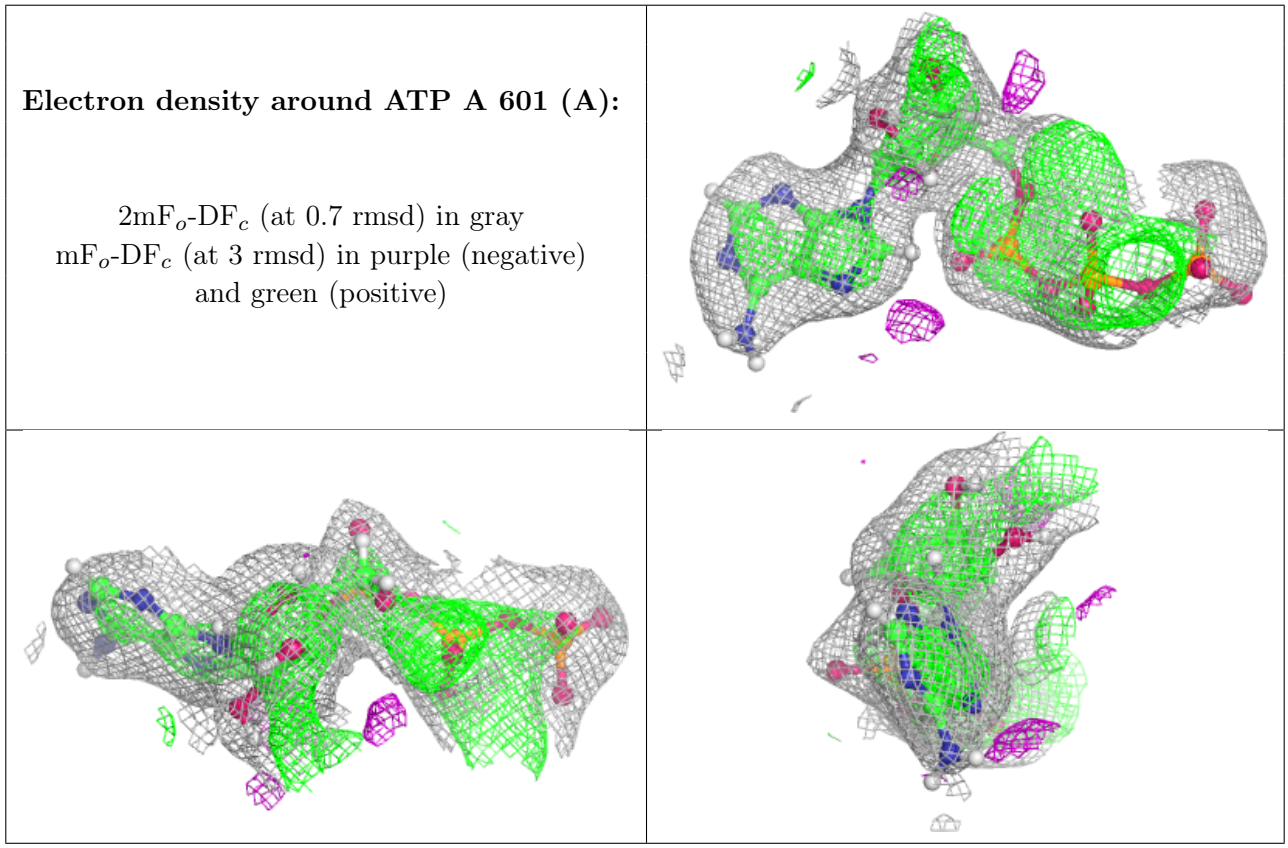
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

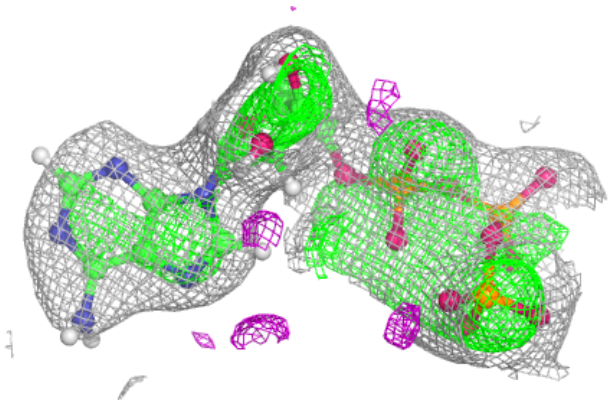
Electron density around ATP A 601 (A):

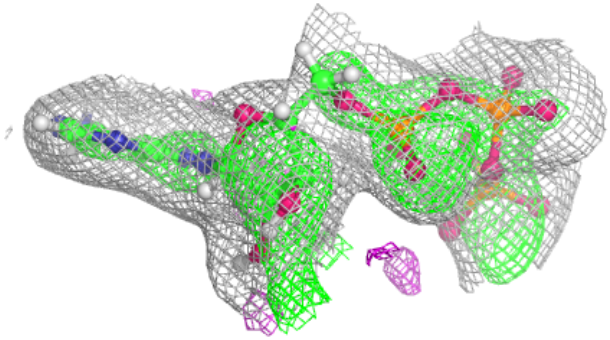
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

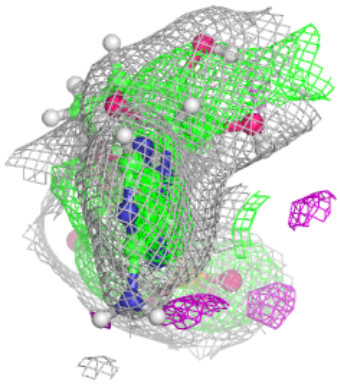


Electron density around ATP A 601 (B):

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

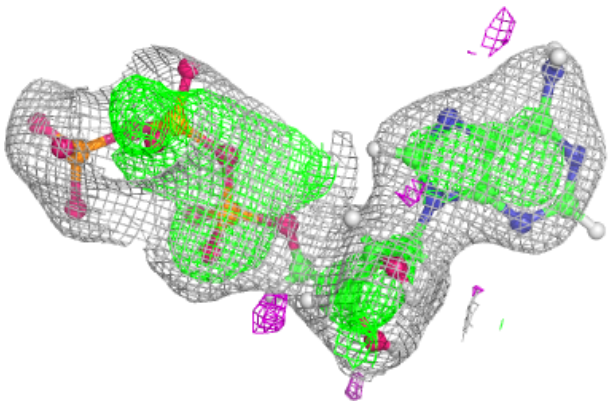


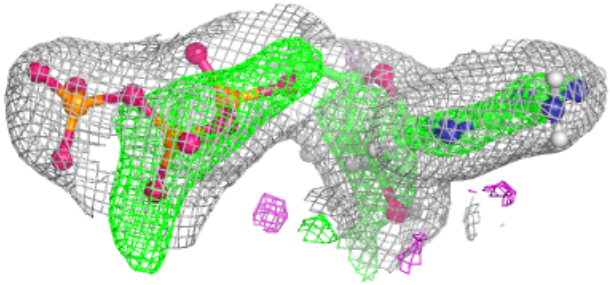


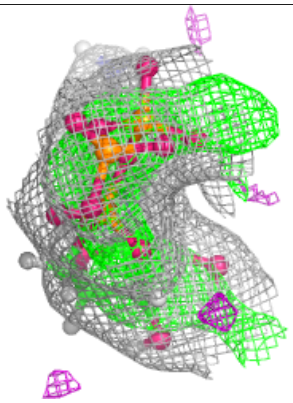


Electron density around ATP B 601 (A):

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

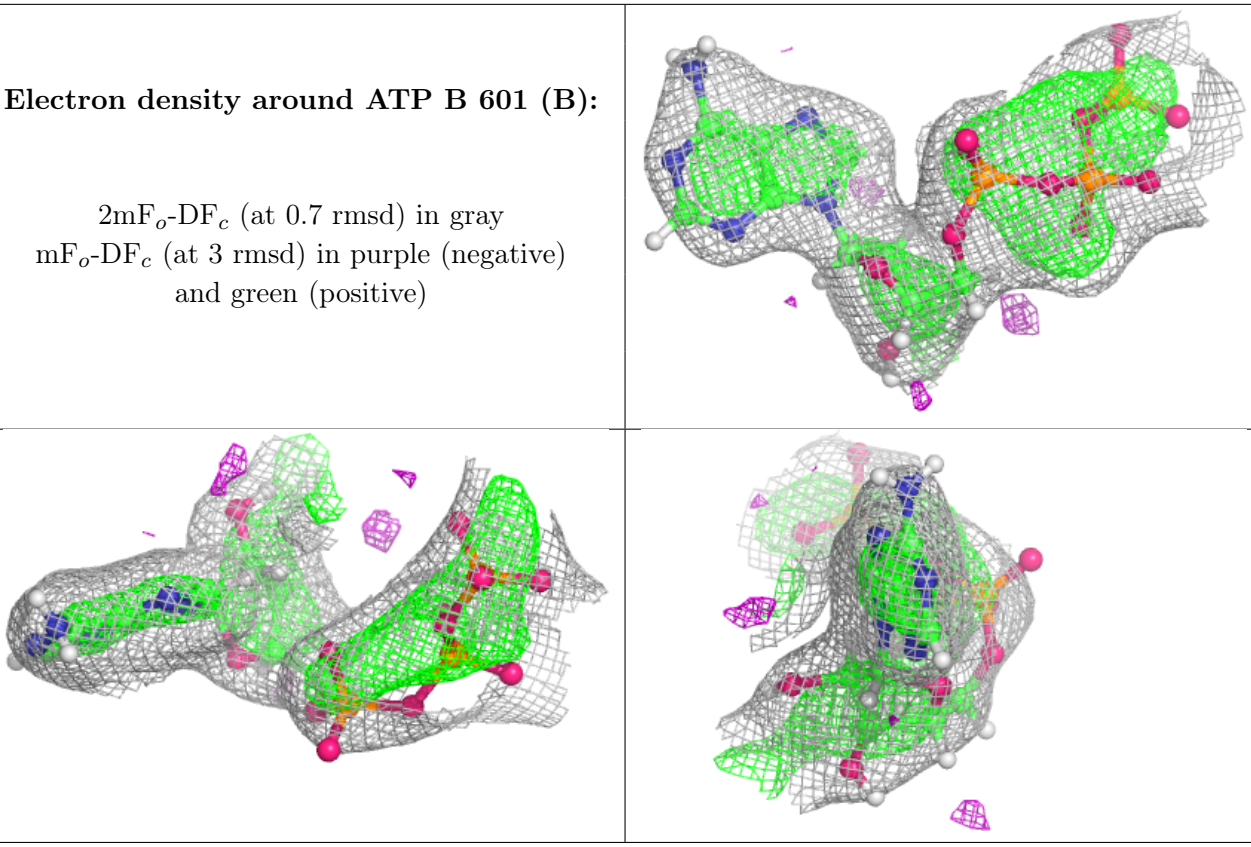






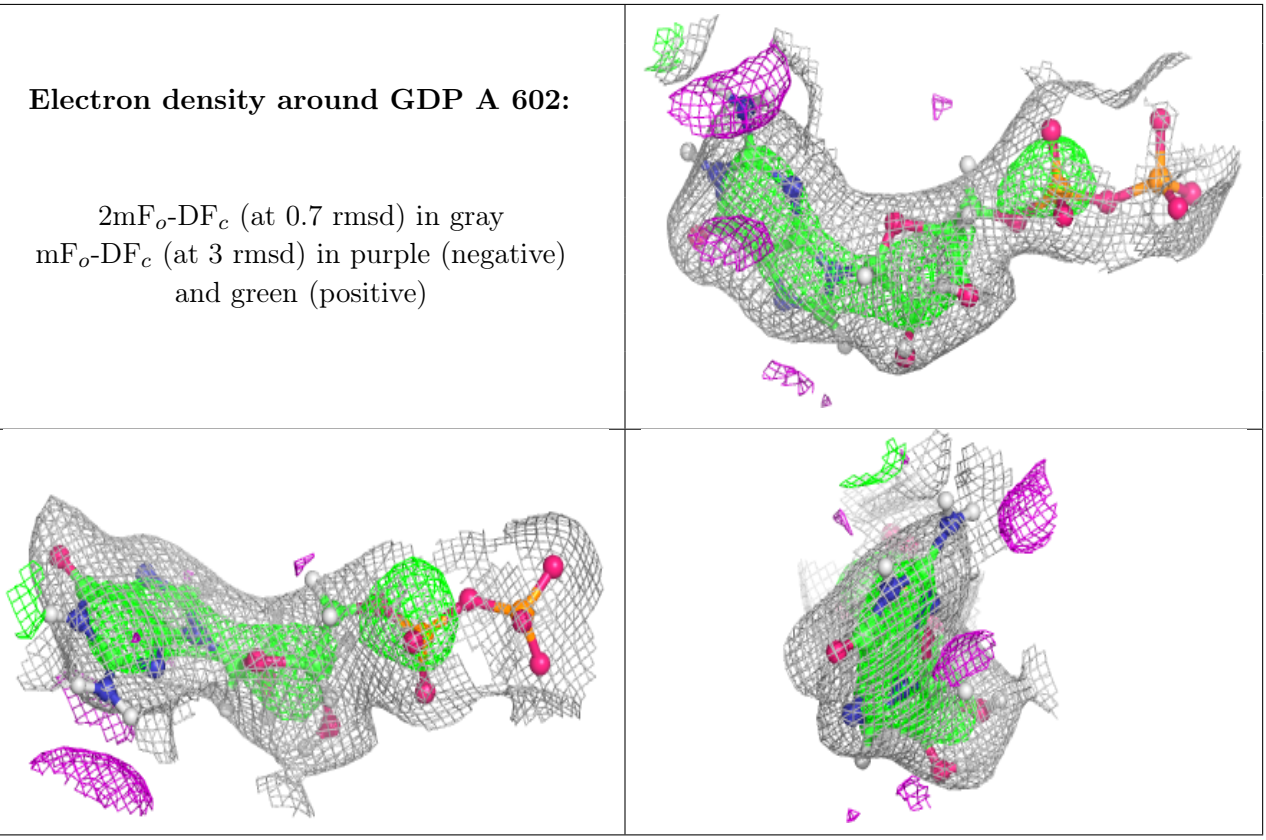
Electron density around ATP B 601 (B):

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



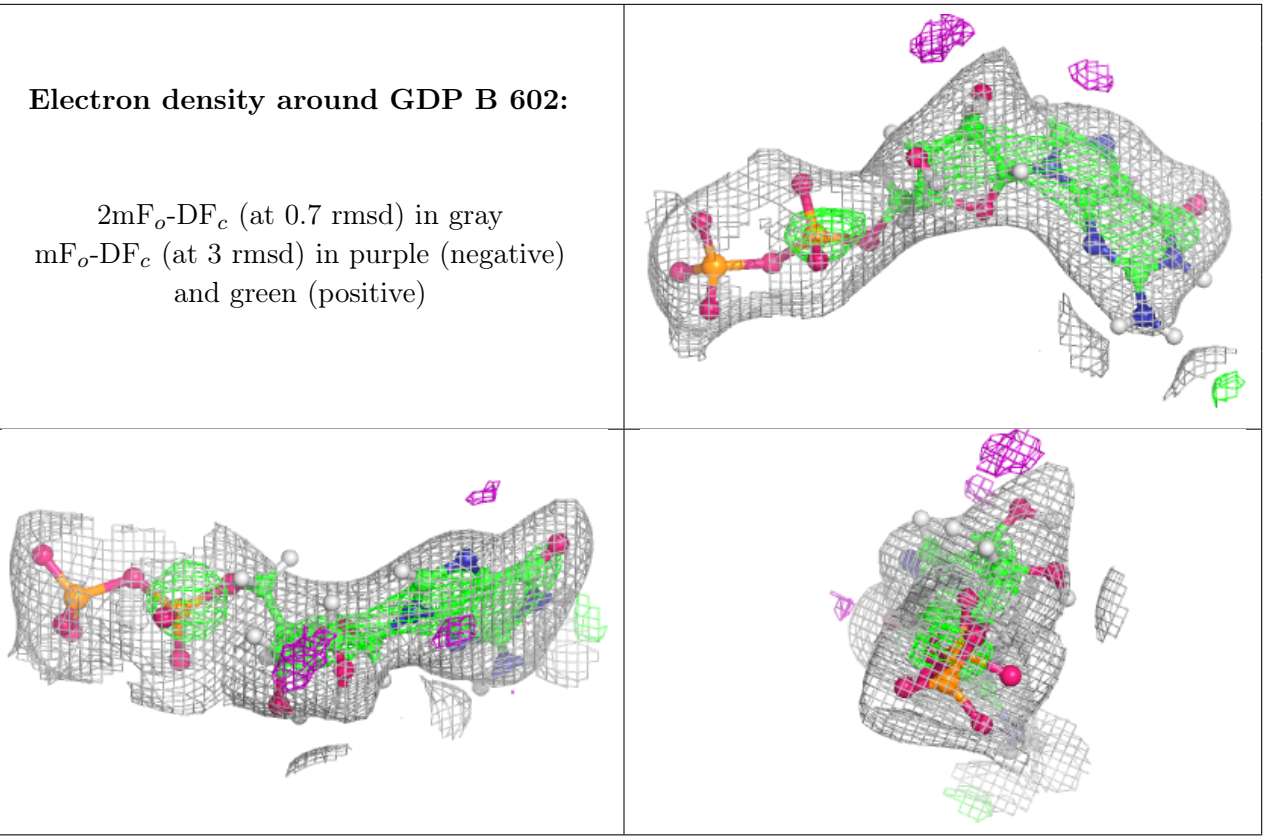
Electron density around GDP A 602:

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



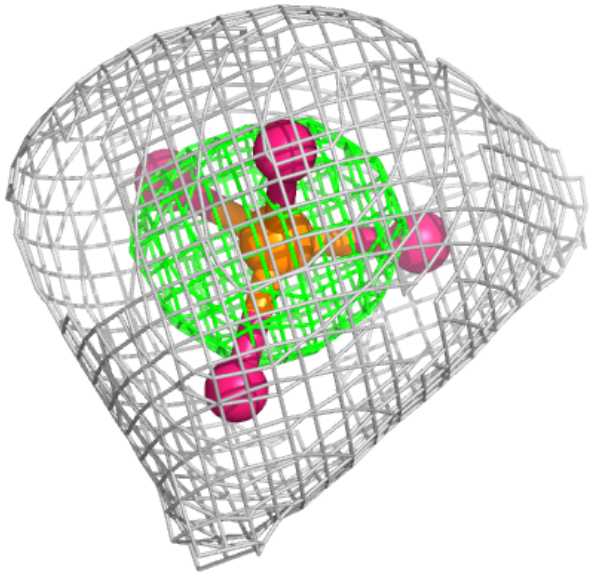
Electron density around GDP B 602:

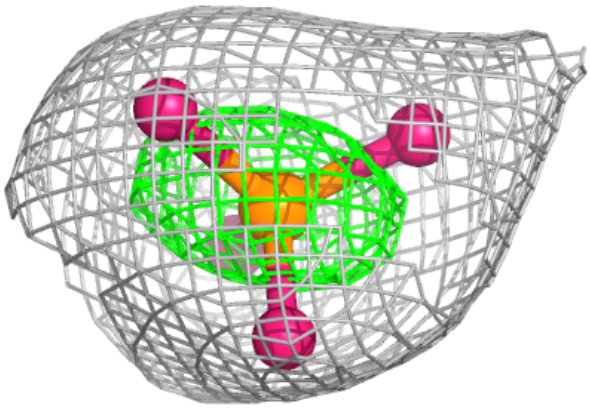
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

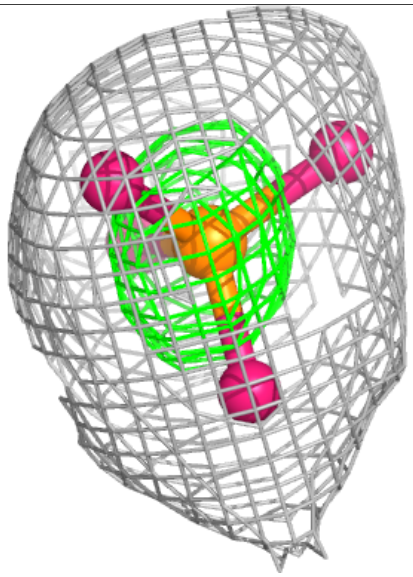


Electron density around PO4 A 603:

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

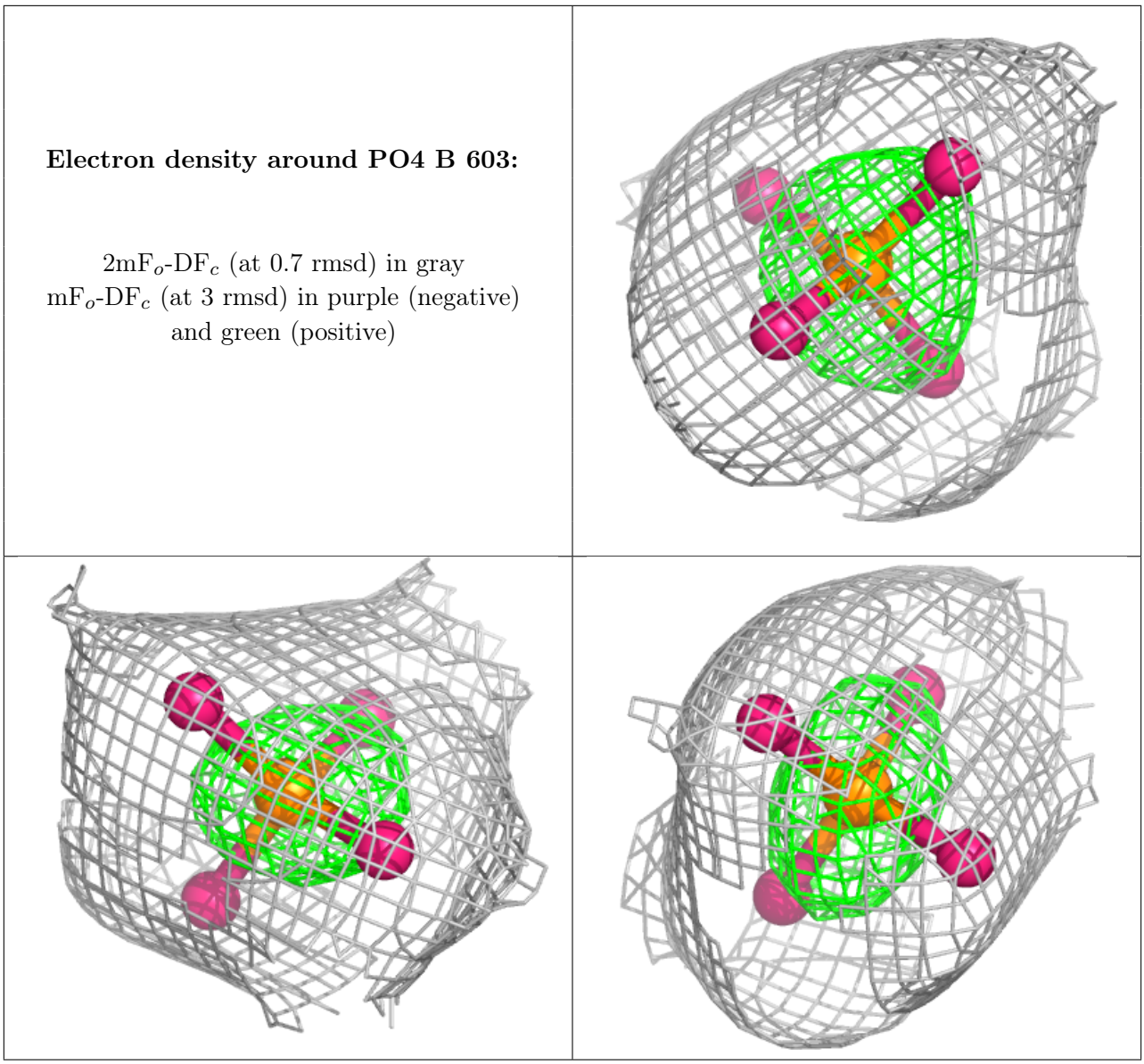






Electron density around PO4 B 603:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.