Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:40 am BST

PDB ID	:	4B1Z
Title	:	Structure of the Phactr1 RPEL domain bound to G-actin
Authors	:	Mouilleron, S.; Wiezlak, M.; O'Reilly, N.; Treisman, R.; McDonald, N.Q.
Deposited on	:	2012-07-12
Resolution	:	3.30 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:

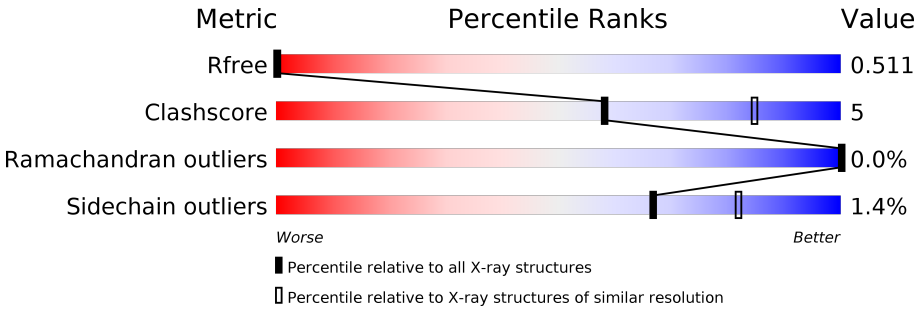
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 on 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	376	80% 10% 11%
1	B	376	85% 10% 5%
1	C	376	88% 10% .
1	D	376	84% 11% 5%
1	E	376	84% 12% 5%
1	F	376	82% 13% 5%
2	M	115	74% 18% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	N	115	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17941 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.

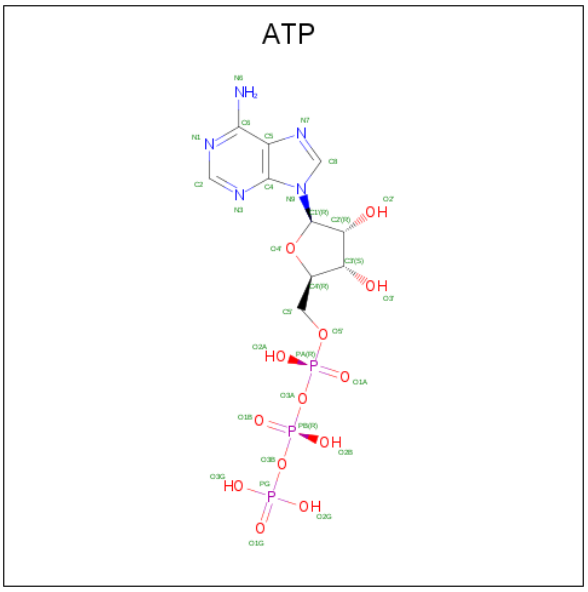
- Molecule 1 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2495	1588	415	474	18			
1	B	357	Total	C	N	O	S	0	0	0
			2711	1721	448	523	19			
1	C	370	Total	C	N	O	S	0	0	0
			2815	1787	476	532	20			
1	D	356	Total	C	N	O	S	0	0	0
			2648	1675	446	508	19			
1	E	359	Total	C	N	O	S	0	0	0
			2682	1701	450	512	19			
1	F	357	Total	C	N	O	S	0	0	0
			2682	1706	444	513	19			

- Molecule 2 is a protein called PHOSPHATASE AND ACTIN REGULATOR 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	110	Total	C	N	O	0	0	0
			846	517	166	163			
2	N	107	Total	C	N	O	0	0	0
			821	505	159	157			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

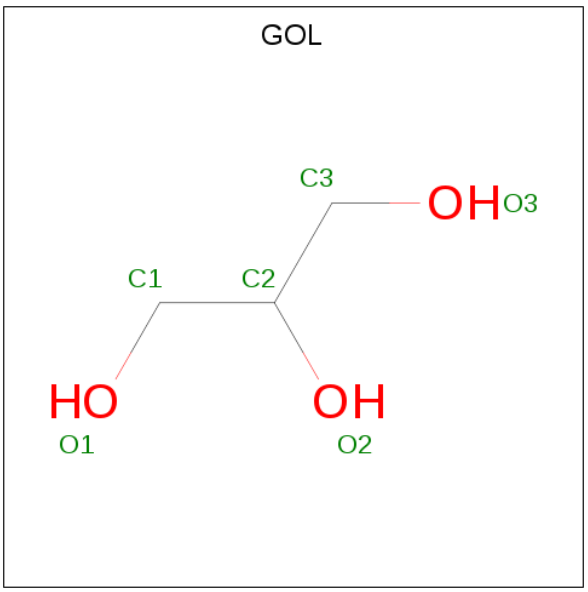


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	N	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

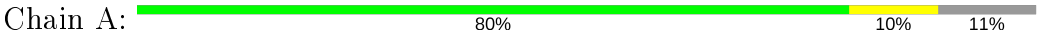
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total O 1 1	0	0

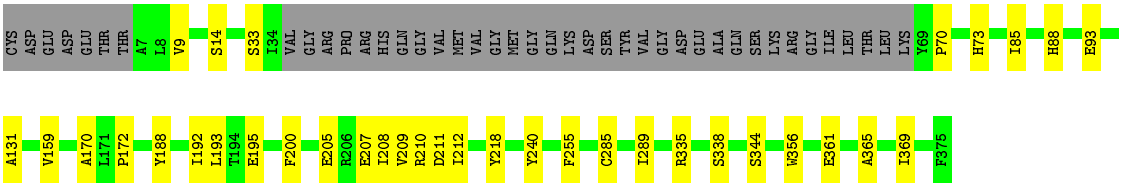
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: ACTIN, ALPHA SKELETAL MUSCLE

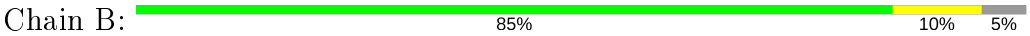
Chain A:

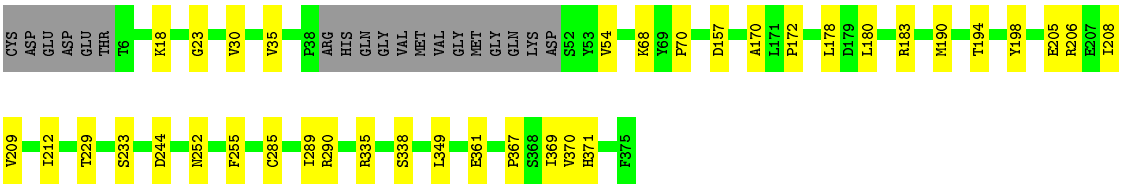




- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

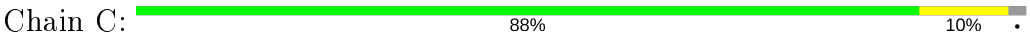
Chain B:

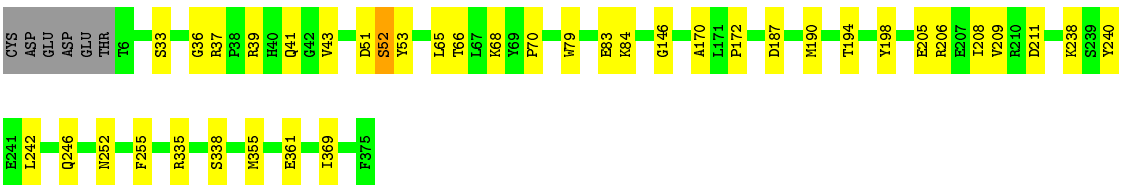




- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

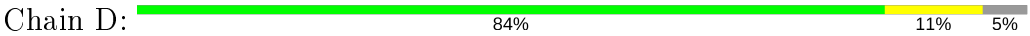
Chain C:

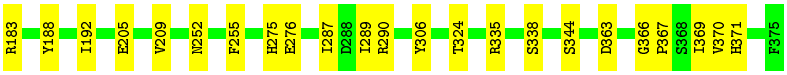




- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

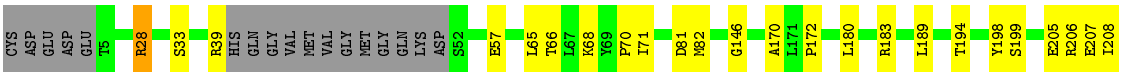
Chain D:

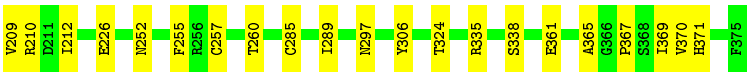




• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain E:



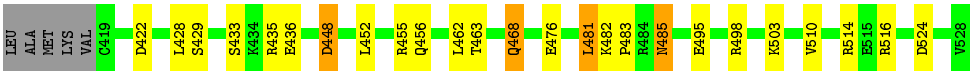


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

Chain F:

• Molecule 2: PHOSPHATASE AND ACTIN REGULATOR 1

Chain M:



• Molecule 2: PHOSPHATASE AND ACTIN REGULATOR 1

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.06Å 142.89Å 184.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.62 – 3.30 74.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (74.62-3.30) 99.4 (74.62-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.34 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.213 , 0.236 0.565 , 0.511	Depositor DCC
R_{free} test set	2580 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å^2)	70.7	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.28$, $< L^2 > = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.50	EDS
Total number of atoms	17941	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: GOL, MG, 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	0.24	0/2552	0.47	0/3480
1	B	0.24	0/2772	0.46	0/3774
1	C	0.24	0/2878	0.47	0/3911
1	D	0.23	0/2706	0.47	0/3685
1	E	0.24	0/2742	0.47	0/3738
1	F	0.25	0/2742	0.48	0/3736
2	M	0.21	0/851	0.43	0/1148
2	N	0.21	0/827	0.41	0/1115
All	All	0.24	0/18070	0.47	0/24587

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	2495	0	2353	19	0
1	B	2711	0	2582	26	0
1	C	2815	0	2724	27	0
1	D	2648	0	2476	26	0
1	E	2682	0	2525	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2682	0	2550	33	0
2	M	846	0	814	13	0
2	N	821	0	787	10	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
3	D	31	0	12	2	0
3	E	31	0	12	1	0
3	F	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	12	0	16	0	0
5	E	6	0	8	1	0
5	F	6	0	8	0	0
5	N	6	0	8	0	0
6	E	1	0	0	0	0
All	All	17941	0	16947	167	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 5.

All (167) 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:E:146:GLY:O	2:N:465:ARG:NH1	2.04	0.89
1:F:371:HIS:HB3	2:N:527:GLU:HG3	1.58	0.84
1:D:62:ARG:HB2	1:D:67:LEU:HD11	1.63	0.80
1:C:41:GLN:O	1:E:28:ARG:NH2	2.14	0.80
1:C:39:ARG:HG2	1:C:66:THR:HG23	1.67	0.77
1:D:157:ASP:OD2	1:D:183:ARG:NH2	2.27	0.66
1:E:70:PRO:HG3	1:E:81:ASP:HB3	1.77	0.65
1:E:39:ARG:HG2	1:E:66:THR:HG23	1.77	0.65
1:C:246:GLN:HG3	1:F:249:THR:OG1	1.97	0.65
1:B:370:VAL:HG13	1:B:371:HIS:HD2	1.62	0.64
2:M:433:SER:HB3	2:M:436:GLU:HG3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:TYR:HD2	1:F:65:LEU:HD21	1.65	0.60
1:D:335:ARG:HA	1:D:338:SER:HB3	1.84	0.60
1:E:370:VAL:HG13	1:E:371:HIS:HD2	1.66	0.59
1:F:53:TYR:CD2	1:F:65:LEU:HD21	2.37	0.59
1:F:190:MET:HG2	1:F:209:VAL:HG21	1.83	0.59
1:D:59:GLN:O	1:D:62:ARG:HB3	2.03	0.58
1:E:199:SER:N	5:E:1378:GOL:O1	2.37	0.58
1:A:335:ARG:HA	1:A:338:SER:HB3	1.85	0.58
1:E:180:LEU:HD21	1:E:260:THR:HG22	1.88	0.56
1:A:14:SER:N	3:A:1376:ATP:O1G	2.26	0.56
1:E:205:GLU:HA	1:E:208:ILE:HG22	1.88	0.55
1:F:59:GLN:O	1:F:62:ARG:HB3	2.07	0.55
1:D:287:ILE:HG12	1:D:290:ARG:NH1	2.23	0.54
1:B:23:GLY:HA2	2:M:455:ARG:NH2	2.22	0.54
1:E:324:THR:HG21	1:F:57:GLU:HA	1.89	0.54
1:B:190:MET:HG2	1:B:209:VAL:HG21	1.89	0.54
1:D:9:VAL:HG21	1:D:344:SER:HA	1.90	0.54
1:F:365:ALA:HB3	1:F:369:ILE:HB	1.89	0.54
1:E:183:ARG:HG2	1:E:206:ARG:HH22	1.72	0.54
2:M:485:ASN:OD1	2:M:485:ASN:N	2.39	0.54
1:E:207:GLU:HG2	1:E:210:ARG:HH21	1.72	0.54
1:F:14:SER:N	3:F:1376:ATP:O1G	2.34	0.54
1:D:146:GLY:HA2	2:N:424:LEU:HD23	1.90	0.54
1:C:53:TYR:HD2	1:C:65:LEU:CD2	2.21	0.53
1:F:70:PRO:HG3	1:F:81:ASP:HB3	1.91	0.53
1:F:241:GLU:OE1	2:N:464:ARG:NH2	2.41	0.53
1:F:194:THR:HA	1:F:198:TYR:O	2.09	0.53
2:M:510:VAL:HG12	2:M:514:ARG:HE	1.74	0.53
1:A:70:PRO:HG2	1:A:85:ILE:HD11	1.89	0.53
1:D:324:THR:HG21	1:E:57:GLU:HA	1.91	0.53
1:C:211:ASP:OD2	1:C:240:TYR:OH	2.22	0.52
1:F:332:PRO:HB2	1:F:334:GLU:OE2	2.10	0.52
1:C:36:GLY:O	1:C:52:SER:HA	2.09	0.52
1:D:367:PRO:O	1:D:370:VAL:HG12	2.10	0.52
1:A:365:ALA:HB3	1:A:369:ILE:HB	1.92	0.52
1:D:33:SER:OG	1:D:33:SER:O	2.28	0.52
1:F:170:ALA:O	1:F:172:PRO:HD3	2.11	0.51
1:C:194:THR:HA	1:C:198:TYR:O	2.10	0.51
1:E:306:TYR:CE1	3:E:1376:ATP:H2	2.29	0.51
1:B:349:LEU:HD13	2:M:463:THR:HG23	1.92	0.51
1:F:205:GLU:O	1:F:209:VAL:HG23	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LYS:O	1:B:70:PRO:HD3	2.11	0.50
1:E:194:THR:HA	1:E:198:TYR:O	2.10	0.50
1:C:205:GLU:O	1:C:209:VAL:HG23	2.12	0.50
1:E:39:ARG:HG3	1:E:65:LEU:HA	1.94	0.50
1:F:33:SER:O	1:F:33:SER:OG	2.28	0.50
1:A:33:SER:OG	1:A:33:SER:O	2.29	0.49
1:E:146:GLY:HA2	2:N:462:LEU:HD23	1.95	0.49
1:C:170:ALA:O	1:C:172:PRO:HD3	2.11	0.49
2:M:495:GLU:OE2	2:M:498:ARG:NH1	2.45	0.49
1:B:194:THR:HA	1:B:198:TYR:O	2.13	0.49
1:E:170:ALA:O	1:E:172:PRO:HD3	2.13	0.49
1:A:285:CYS:HB3	1:A:289:ILE:HD11	1.95	0.48
1:B:18:LYS:HG3	1:B:30:VAL:HG22	1.94	0.48
1:F:18:LYS:HG3	1:F:30:VAL:HG22	1.94	0.48
1:E:33:SER:OG	1:E:33:SER:O	2.28	0.48
1:D:289:ILE:HD11	2:N:442:ILE:HG12	1.94	0.48
1:F:214:GLU:O	2:N:478:ARG:NH1	2.39	0.48
1:D:70:PRO:HG3	1:D:81:ASP:HB3	1.95	0.48
1:E:252:ASN:HA	1:E:255:PHE:CE1	2.49	0.48
1:B:170:ALA:O	1:B:172:PRO:HD3	2.14	0.48
1:D:14:SER:N	3:D:1376:ATP:O1G	2.32	0.48
1:C:190:MET:HG2	1:C:209:VAL:HG21	1.94	0.47
1:F:349:LEU:HD11	2:N:500:LEU:HD23	1.95	0.47
1:D:188:TYR:O	1:D:192:ILE:HG12	2.14	0.47
1:E:183:ARG:HG2	1:E:206:ARG:NH2	2.29	0.47
1:E:208:ILE:O	1:E:212:ILE:HG13	2.14	0.47
1:F:193:LEU:HD21	1:F:250:ILE:HG13	1.97	0.47
1:C:146:GLY:O	2:M:503:LYS:NZ	2.47	0.47
2:M:452:LEU:O	2:M:456:GLN:HG2	2.14	0.47
1:D:68:LYS:O	1:D:70:PRO:HD3	2.15	0.47
1:A:170:ALA:O	1:A:172:PRO:HD3	2.15	0.46
1:B:229:THR:HG23	1:D:367:PRO:HD2	1.96	0.46
2:N:485:ASN:ND2	2:N:488:GLU:OE1	2.48	0.46
1:E:285:CYS:HB3	1:E:289:ILE:HD11	1.97	0.46
1:E:370:VAL:HG13	1:E:371:HIS:CD2	2.49	0.46
1:E:205:GLU:O	1:E:209:VAL:HG23	2.15	0.46
1:F:367:PRO:O	1:F:370:VAL:HG12	2.16	0.46
2:M:482:LYS:HA	2:M:483:PRO:HD3	1.84	0.46
1:C:36:GLY:HA3	1:C:65:LEU:HD13	1.98	0.46
1:F:252:ASN:HA	1:F:255:PHE:CE1	2.50	0.46
1:A:205:GLU:O	1:A:209:VAL:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:TYR:HD2	1:D:65:LEU:HD21	1.81	0.46
1:A:208:ILE:O	1:A:212:ILE:HG13	2.16	0.45
1:F:71:ILE:HD11	1:F:82:MET:SD	2.55	0.45
1:B:361:GLU:HB3	1:B:369:ILE:HD13	1.97	0.45
1:D:205:GLU:O	1:D:209:VAL:HG23	2.16	0.45
1:B:370:VAL:HG13	1:B:371:HIS:CD2	2.47	0.45
1:C:68:LYS:O	1:C:70:PRO:HD3	2.16	0.45
1:F:68:LYS:O	1:F:70:PRO:HD3	2.17	0.45
1:B:367:PRO:O	1:B:370:VAL:HG12	2.17	0.45
1:D:170:ALA:O	1:D:172:PRO:HD3	2.16	0.45
1:F:208:ILE:O	1:F:212:ILE:HG13	2.16	0.45
1:B:178:LEU:HG	1:B:180:LEU:HB3	1.98	0.45
1:F:366:GLY:O	1:F:369:ILE:HG22	2.17	0.45
2:M:448:ASP:N	2:M:448:ASP:OD1	2.49	0.45
1:A:73:HIS:HA	1:A:159:VAL:HB	1.97	0.45
1:A:131:ALA:HB1	1:A:356:TRP:HB3	1.99	0.45
1:D:252:ASN:HA	1:D:255:PHE:CE1	2.52	0.44
1:C:361:GLU:HB3	1:C:369:ILE:HD13	1.99	0.44
1:B:233:SER:HB2	1:D:363:ASP:HA	1.99	0.44
1:A:9:VAL:HG21	1:A:344:SER:HA	1.99	0.44
1:C:33:SER:O	1:C:33:SER:OG	2.29	0.44
1:C:238:LYS:HD3	2:M:468:GLN:NE2	2.33	0.44
2:M:476:GLU:HG2	2:M:481:LEU:HB3	1.99	0.44
1:D:275:HIS:CE1	1:D:276:GLU:HG3	2.53	0.44
1:A:211:ASP:OD2	1:A:240:TYR:OH	2.16	0.44
1:F:37:ARG:O	1:F:65:LEU:HB2	2.18	0.44
1:B:335:ARG:HA	1:B:338:SER:HB3	1.99	0.44
1:C:37:ARG:HH22	1:C:84:LYS:HE3	1.83	0.44
1:C:51:ASP:O	1:C:52:SER:OG	2.26	0.44
1:C:187:ASP:OD1	1:C:206:ARG:NH2	2.40	0.43
1:C:53:TYR:HD2	1:C:65:LEU:HD21	1.83	0.43
1:E:189:LEU:HD13	1:E:257:CYS:HB2	1.99	0.43
1:E:71:ILE:HD11	1:E:82:MET:SD	2.59	0.43
1:B:35:VAL:HG22	1:B:54:VAL:HG22	2.00	0.43
1:C:208:ILE:HG21	1:C:242:LEU:HD22	1.99	0.43
1:E:324:THR:HG21	1:F:57:GLU:CA	2.48	0.43
1:F:285:CYS:HB3	1:F:289:ILE:HD11	2.02	0.42
1:C:252:ASN:HA	1:C:255:PHE:CE1	2.53	0.42
1:E:226:GLU:HB3	1:E:255:PHE:CE2	2.54	0.42
1:E:335:ARG:HA	1:E:338:SER:HB3	2.01	0.42
1:D:116:ARG:HH12	1:D:371:HIS:HA	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLU:O	1:B:209:VAL:HG23	2.19	0.42
1:B:285:CYS:HB3	1:B:289:ILE:HD11	2.02	0.42
1:B:252:ASN:HA	1:B:255:PHE:CE1	2.54	0.42
1:B:349:LEU:HD11	2:M:462:LEU:HD23	2.02	0.42
1:C:335:ARG:HA	1:C:338:SER:HB3	2.01	0.42
1:F:9:VAL:HG21	1:F:344:SER:HA	2.02	0.42
1:A:88:HIS:CD2	1:A:93:GLU:HG2	2.55	0.42
1:F:124:PHE:CZ	1:F:132:MET:HG3	2.55	0.42
1:D:366:GLY:O	1:D:369:ILE:HG22	2.20	0.41
1:E:68:LYS:O	1:E:70:PRO:HD3	2.20	0.41
1:B:157:ASP:OD1	3:B:1376:ATP:O3'	2.30	0.41
1:C:79:TRP:O	1:C:83:GLU:HG3	2.20	0.41
1:E:365:ALA:HB3	1:E:369:ILE:HB	2.02	0.41
1:D:18:LYS:HG3	1:D:30:VAL:HG22	2.02	0.41
1:B:190:MET:HG3	1:B:209:VAL:HG11	2.01	0.41
1:D:306:TYR:CE1	3:D:1376:ATP:H2	2.38	0.41
1:E:367:PRO:O	1:E:370:VAL:HG12	2.20	0.41
2:N:464:ARG:O	2:N:467:SER:OG	2.25	0.41
1:B:285:CYS:O	1:B:290:ARG:NH2	2.42	0.41
1:F:338:SER:HA	1:F:341:ILE:HD12	2.03	0.41
1:A:207:GLU:CD	1:A:210:ARG:HH21	2.24	0.41
1:C:65:LEU:O	1:C:65:LEU:HD12	2.20	0.41
1:F:193:LEU:HD23	1:F:193:LEU:HA	1.95	0.41
1:A:193:LEU:HD13	1:A:200:PHE:CE2	2.56	0.41
1:A:218:TYR:O	1:A:255:PHE:HA	2.21	0.41
1:B:208:ILE:O	1:B:212:ILE:HG13	2.21	0.41
1:B:244:ASP:N	1:B:244:ASP:OD1	2.53	0.41
1:C:43:VAL:HG22	1:E:28:ARG:HD2	2.01	0.41
1:E:361:GLU:HB3	1:E:369:ILE:HD13	2.03	0.41
1:A:361:GLU:HB3	1:A:369:ILE:HD13	2.02	0.41
1:C:53:TYR:CD2	1:C:65:LEU:HD21	2.56	0.41
1:A:188:TYR:O	1:A:192:ILE:HG12	2.20	0.40
1:B:183:ARG:HG2	1:B:206:ARG:NH2	2.36	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	331/376 (88%)	326 (98%)	5 (2%)	0	100 100
1	B	353/376 (94%)	347 (98%)	6 (2%)	0	100 100
1	C	368/376 (98%)	359 (98%)	8 (2%)	1 (0%)	41 71
1	D	352/376 (94%)	346 (98%)	6 (2%)	0	100 100
1	E	355/376 (94%)	348 (98%)	7 (2%)	0	100 100
1	F	353/376 (94%)	346 (98%)	7 (2%)	0	100 100
2	M	108/115 (94%)	105 (97%)	3 (3%)	0	100 100
2	N	105/115 (91%)	102 (97%)	3 (3%)	0	100 100
All	All	2325/2486 (94%)	2279 (98%)	45 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	SER

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	251/319 (79%)	250 (100%)	1 (0%)	91 95
1	B	281/319 (88%)	281 (100%)	0	100 100
1	C	292/319 (92%)	291 (100%)	1 (0%)	92 96
1	D	264/319 (83%)	262 (99%)	2 (1%)	81 89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	270/319 (85%)	268 (99%)	2 (1%)	84 90
1	F	274/319 (86%)	273 (100%)	1 (0%)	91 95
2	M	83/111 (75%)	73 (88%)	10 (12%)	5 20
2	N	80/111 (72%)	71 (89%)	9 (11%)	6 22
All	All	1795/2136 (84%)	1769 (99%)	26 (1%)	67 82

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLU
1	C	355	MET
1	D	61	LYS
1	D	62	ARG
1	E	28	ARG
1	E	297	ASN
1	F	62	ARG
2	M	422	ASP
2	M	428	LEU
2	M	429	SER
2	M	435	ARG
2	M	448	ASP
2	M	468	GLN
2	M	481	LEU
2	M	485	ASN
2	M	516	ARG
2	M	524	ASP
2	N	424	LEU
2	N	428	LEU
2	N	435	ARG
2	N	439	GLU
2	N	448	ASP
2	N	452	LEU
2	N	461	LYS
2	N	462	LEU
2	N	527	GLU

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

Mol	Chain	Res	Type
1	A	88	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	371	HIS
1	E	371	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	GOL	A	1379	-	5,5,5	0.37	0	5,5,5	0.28	0
3	ATP	C	1376	4	26,33,33	0.92	1 (3%)	31,52,52	1.43	5 (16%)
5	GOL	B	1378	-	5,5,5	0.36	0	5,5,5	0.22	0
5	GOL	C	1378	-	5,5,5	0.38	0	5,5,5	0.30	0
5	GOL	F	1378	-	5,5,5	0.38	0	5,5,5	0.22	0
5	GOL	A	1378	-	5,5,5	0.38	0	5,5,5	0.21	0
5	GOL	E	1378	-	5,5,5	0.36	0	5,5,5	0.31	0
5	GOL	N	1529	-	5,5,5	0.37	0	5,5,5	0.29	0
3	ATP	A	1376	4	26,33,33	0.92	1 (3%)	31,52,52	1.44	5 (16%)
3	ATP	B	1376	4	26,33,33	0.90	1 (3%)	31,52,52	1.48	5 (16%)
3	ATP	E	1376	4	26,33,33	0.93	1 (3%)	31,52,52	1.38	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ATP	F	1376	4	26,33,33	0.91	1 (3%)	31,52,52	1.40	5 (16%)
3	ATP	D	1376	4	26,33,33	0.93	1 (3%)	31,52,52	1.40	5 (16%)
5	GOL	C	1379	-	5,5,5	0.37	0	5,5,5	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1379	-	-	0/4/4/4	-
3	ATP	C	1376	4	-	0/18/38/38	0/3/3/3
5	GOL	B	1378	-	-	2/4/4/4	-
5	GOL	C	1378	-	-	2/4/4/4	-
5	GOL	F	1378	-	-	2/4/4/4	-
5	GOL	A	1378	-	-	2/4/4/4	-
5	GOL	E	1378	-	-	2/4/4/4	-
5	GOL	N	1529	-	-	2/4/4/4	-
3	ATP	A	1376	4	-	0/18/38/38	0/3/3/3
3	ATP	B	1376	4	-	2/18/38/38	0/3/3/3
3	ATP	E	1376	4	-	4/18/38/38	0/3/3/3
3	ATP	F	1376	4	-	0/18/38/38	0/3/3/3
3	ATP	D	1376	4	-	0/18/38/38	0/3/3/3
5	GOL	C	1379	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1376	ATP	C5-C4	2.50	1.47	1.40
3	D	1376	ATP	C5-C4	2.48	1.47	1.40
3	C	1376	ATP	C5-C4	2.48	1.47	1.40
3	A	1376	ATP	C5-C4	2.46	1.47	1.40
3	F	1376	ATP	C5-C4	2.45	1.47	1.40
3	B	1376	ATP	C5-C4	2.43	1.47	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1376	ATP	N3-C2-N1	-3.30	123.52	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1376	ATP	N3-C2-N1	-3.26	123.58	128.68
3	C	1376	ATP	N3-C2-N1	-3.23	123.63	128.68
3	B	1376	ATP	PA-O3A-PB	-3.17	121.94	132.83
3	A	1376	ATP	N3-C2-N1	-3.16	123.73	128.68
3	D	1376	ATP	N3-C2-N1	-3.07	123.89	128.68
3	B	1376	ATP	C3'-C2'-C1'	2.90	105.35	100.98
3	C	1376	ATP	PA-O3A-PB	-2.88	122.95	132.83
3	B	1376	ATP	C4-C5-N7	-2.87	106.41	109.40
3	A	1376	ATP	PA-O3A-PB	-2.82	123.15	132.83
3	E	1376	ATP	C4-C5-N7	-2.81	106.47	109.40
3	A	1376	ATP	C3'-C2'-C1'	2.80	105.19	100.98
3	D	1376	ATP	PA-O3A-PB	-2.79	123.24	132.83
3	C	1376	ATP	C4-C5-N7	-2.74	106.54	109.40
3	E	1376	ATP	PA-O3A-PB	-2.69	123.60	132.83
3	A	1376	ATP	PB-O3B-PG	-2.69	123.61	132.83
3	E	1376	ATP	N3-C2-N1	-2.69	124.48	128.68
3	F	1376	ATP	C4-C5-N7	-2.68	106.61	109.40
3	B	1376	ATP	PB-O3B-PG	-2.68	123.64	132.83
3	C	1376	ATP	PB-O3B-PG	-2.66	123.71	132.83
3	D	1376	ATP	C4-C5-N7	-2.63	106.66	109.40
3	E	1376	ATP	C3'-C2'-C1'	2.63	104.93	100.98
3	A	1376	ATP	C4-C5-N7	-2.61	106.68	109.40
3	E	1376	ATP	PB-O3B-PG	-2.60	123.91	132.83
3	F	1376	ATP	C3'-C2'-C1'	2.54	104.80	100.98
3	C	1376	ATP	C3'-C2'-C1'	2.52	104.78	100.98
3	D	1376	ATP	C3'-C2'-C1'	2.52	104.78	100.98
3	F	1376	ATP	PA-O3A-PB	-2.51	124.20	132.83
3	D	1376	ATP	PB-O3B-PG	-2.46	124.40	132.83
3	F	1376	ATP	PB-O3B-PG	-2.43	124.48	132.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	N	1529	GOL	C1-C2-C3-O3
5	B	1378	GOL	C1-C2-C3-O3
5	C	1378	GOL	C1-C2-C3-O3
5	F	1378	GOL	C1-C2-C3-O3
5	A	1378	GOL	C1-C2-C3-O3
3	E	1376	ATP	C5'-O5'-PA-O2A
5	C	1379	GOL	C1-C2-C3-O3
5	C	1378	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1378	GOL	O2-C2-C3-O3
5	C	1379	GOL	O2-C2-C3-O3
5	N	1529	GOL	O2-C2-C3-O3
5	F	1378	GOL	O2-C2-C3-O3
5	E	1378	GOL	O2-C2-C3-O3
3	E	1376	ATP	C5'-O5'-PA-O3A
5	C	1379	GOL	O1-C1-C2-O2
3	B	1376	ATP	PG-O3B-PB-O1B
5	E	1378	GOL	C1-C2-C3-O3
5	B	1378	GOL	O2-C2-C3-O3
5	C	1379	GOL	O1-C1-C2-C3
3	E	1376	ATP	C3'-C4'-C5'-O5'
3	B	1376	ATP	PG-O3B-PB-O2B
3	E	1376	ATP	C5'-O5'-PA-O1A

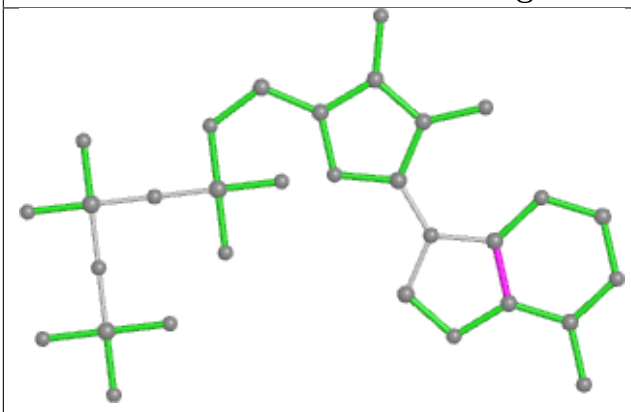
There are no ring outliers.

6 monomers are involved in 7 short contacts:

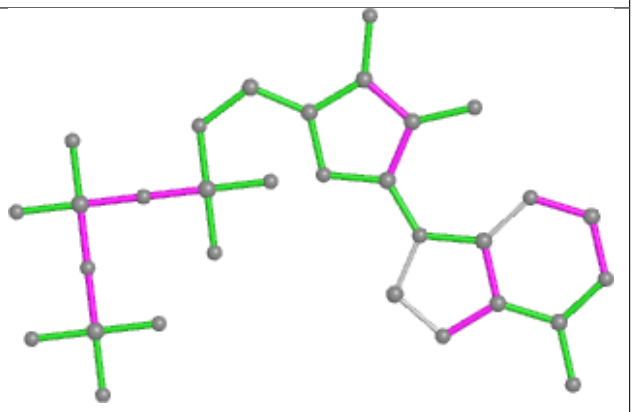
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1378	GOL	1	0
3	A	1376	ATP	1	0
3	B	1376	ATP	1	0
3	E	1376	ATP	1	0
3	F	1376	ATP	1	0
3	D	1376	ATP	2	0

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.

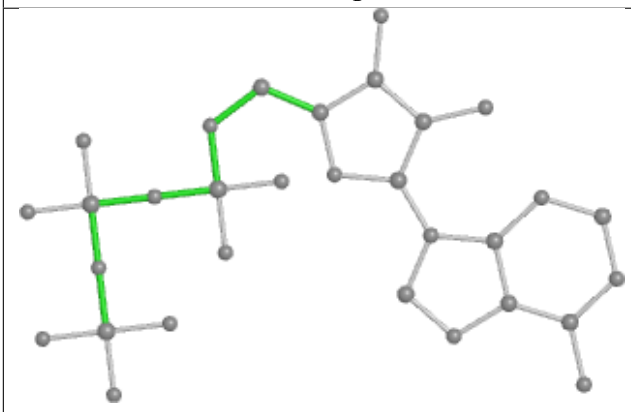
Ligand ATP C 1376



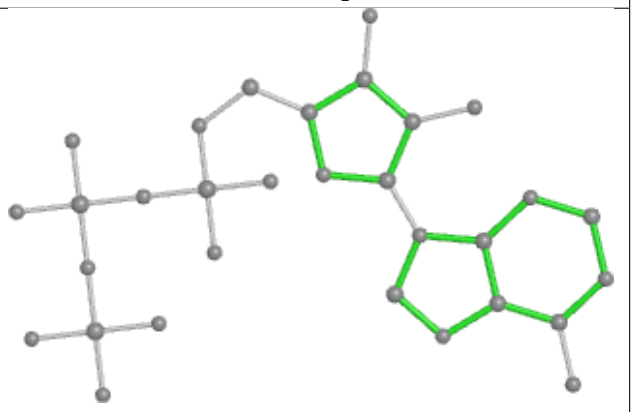
Bond lengths



Bond angles

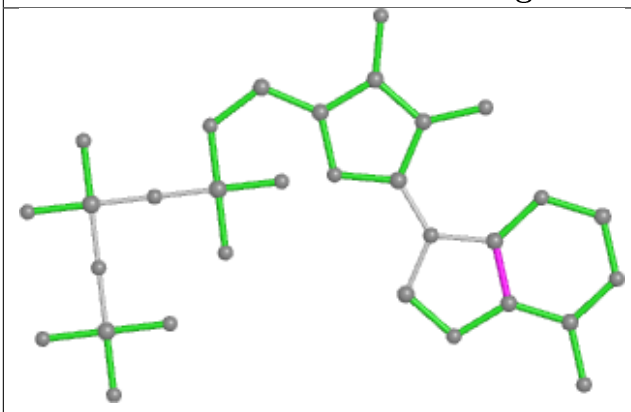


Torsions

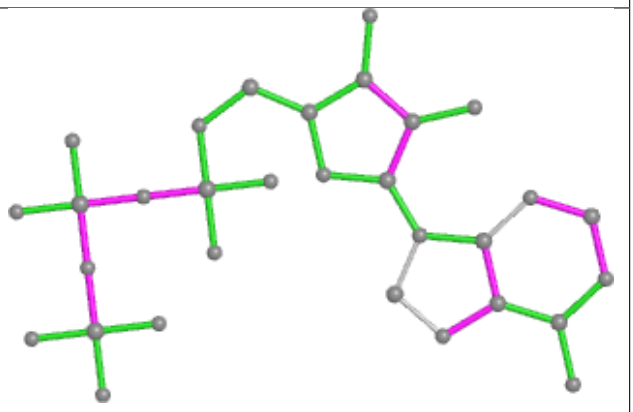


Rings

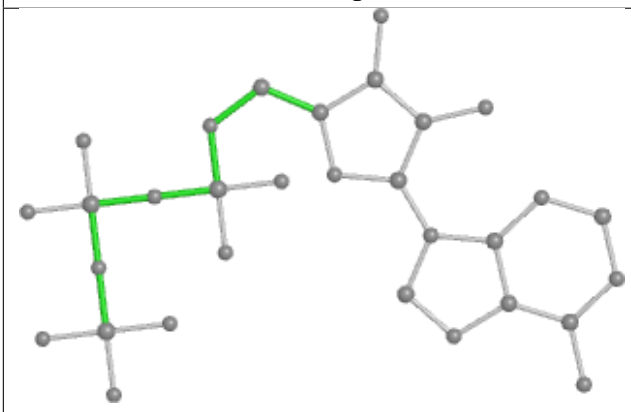
Ligand ATP A 1376



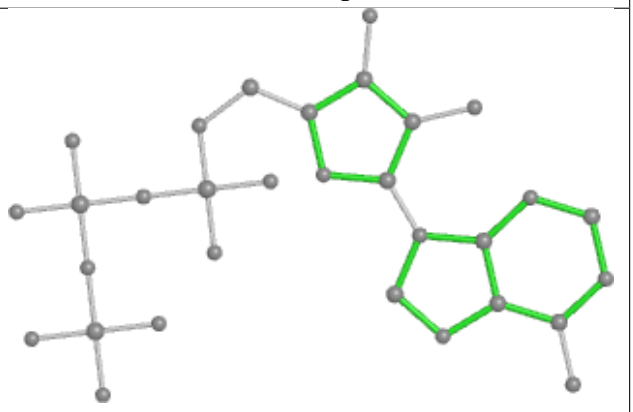
Bond lengths



Bond angles

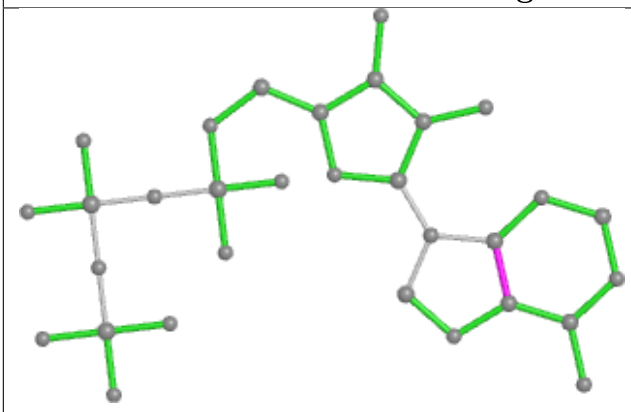


Torsions

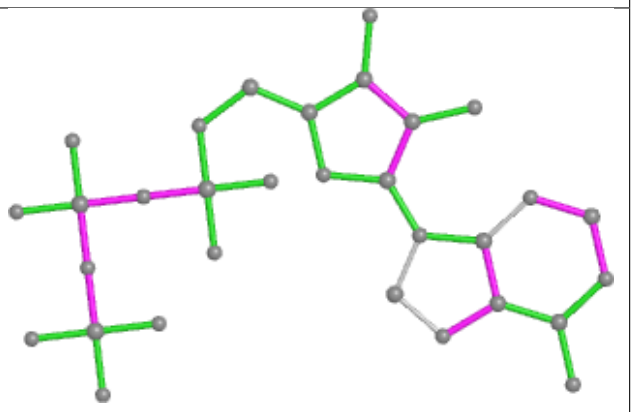


Rings

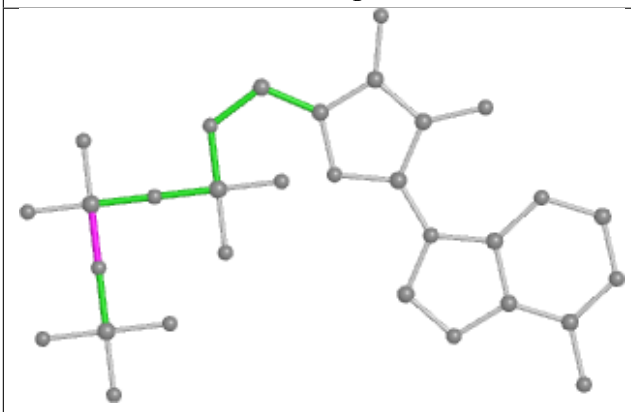
Ligand ATP B 1376



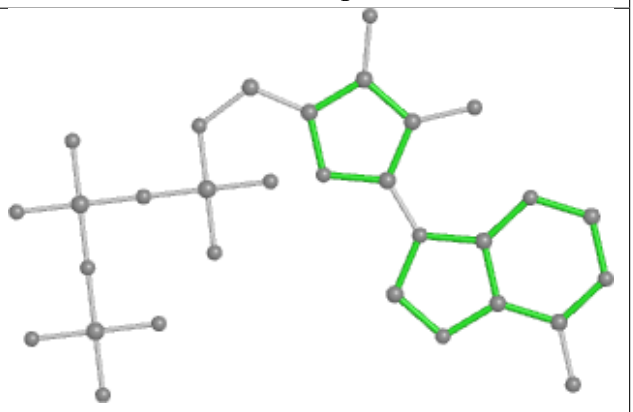
Bond lengths



Bond angles

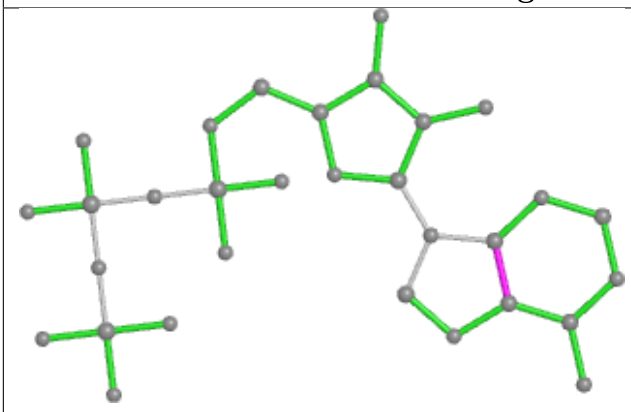


Torsions

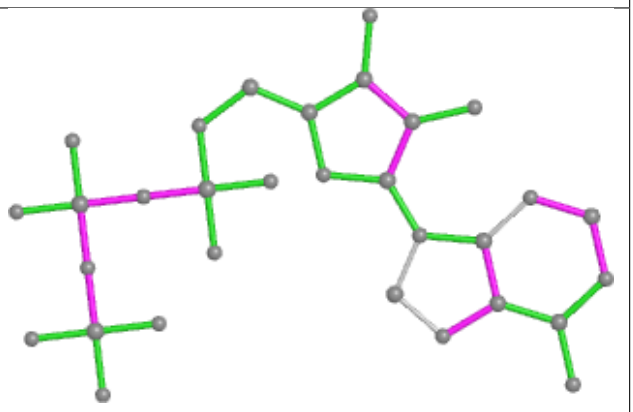


Rings

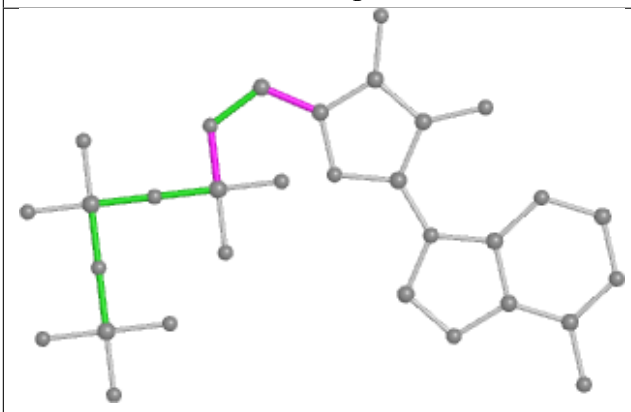
Ligand ATP E 1376



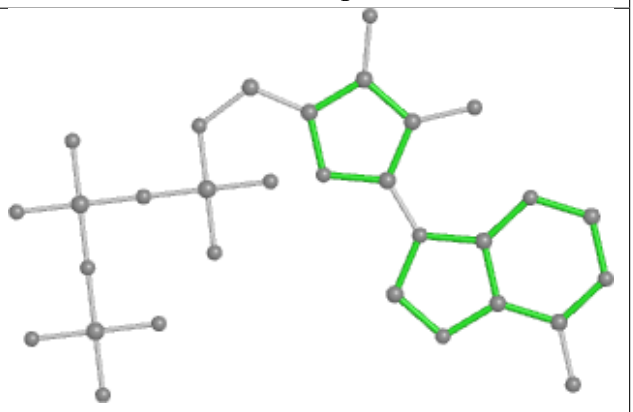
Bond lengths



Bond angles

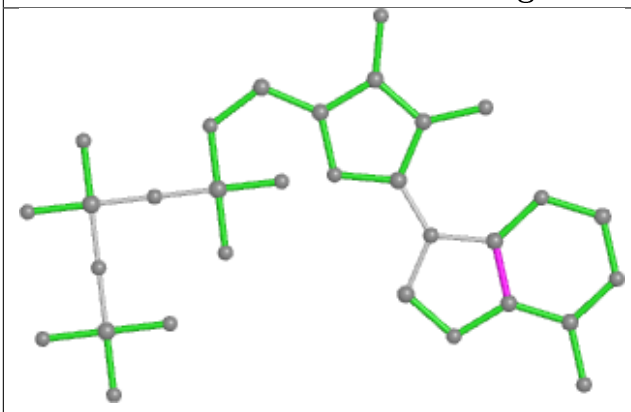


Torsions

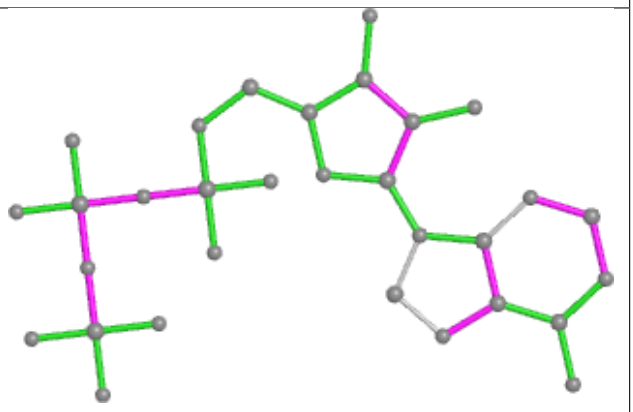


Rings

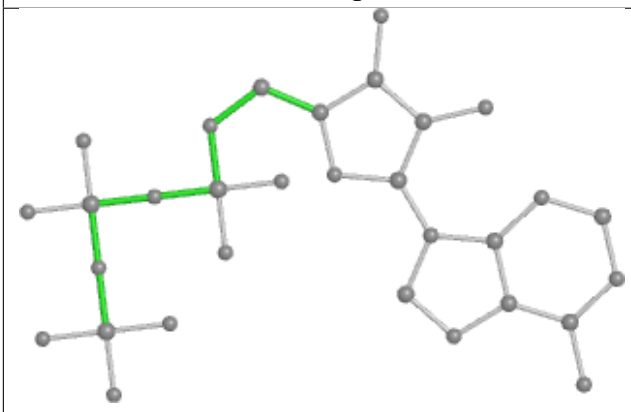
Ligand ATP F 1376



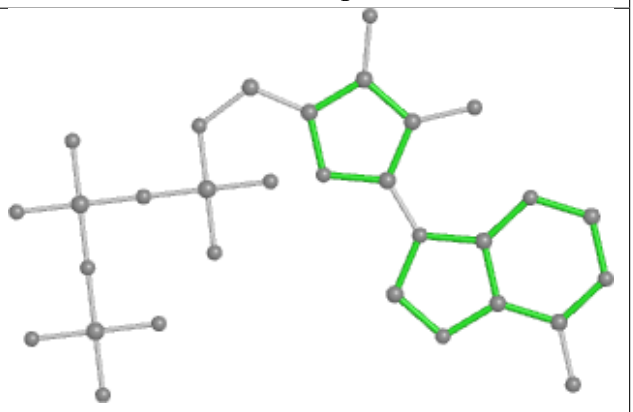
Bond lengths



Bond angles

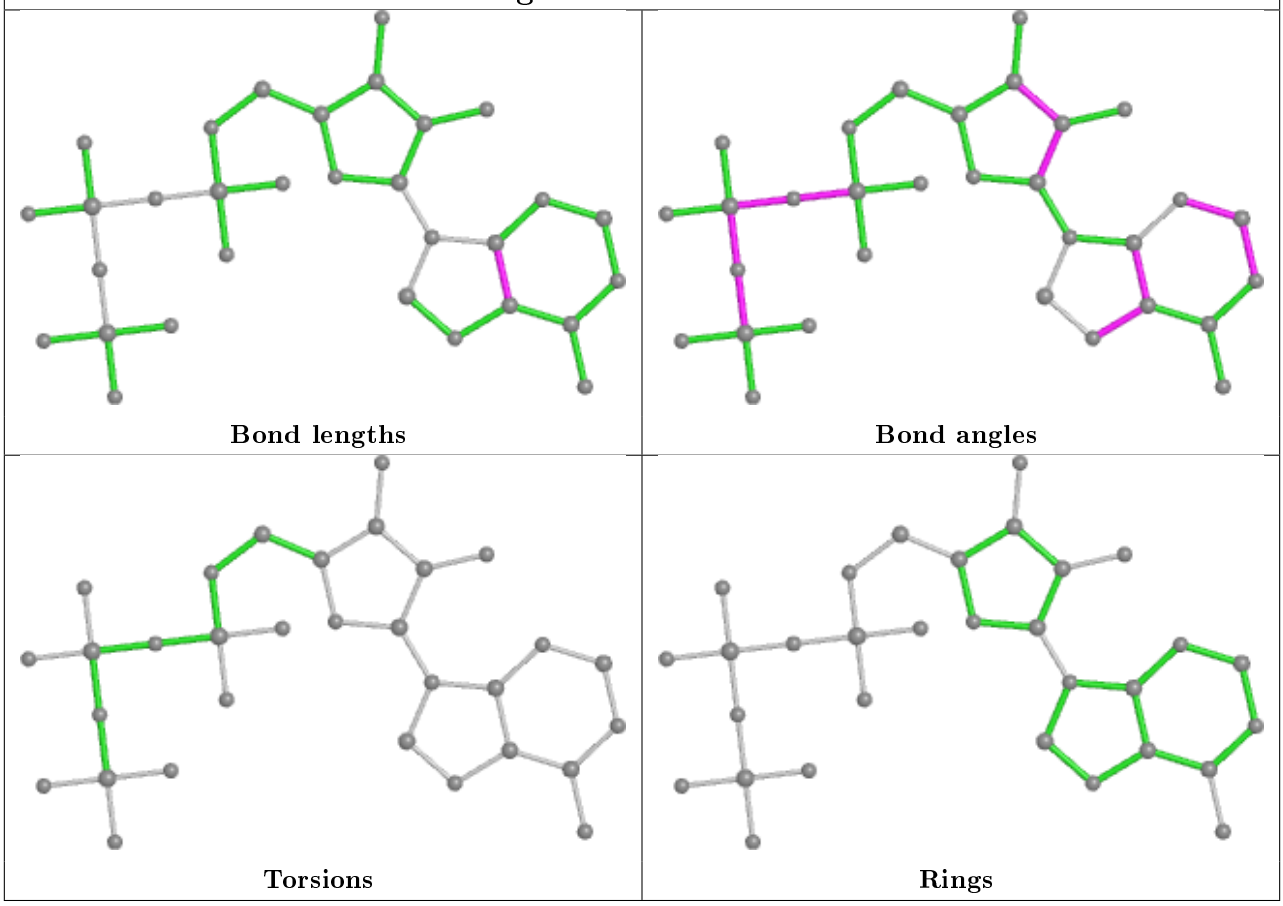


Torsions



Rings

Ligand ATP D 1376



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

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.

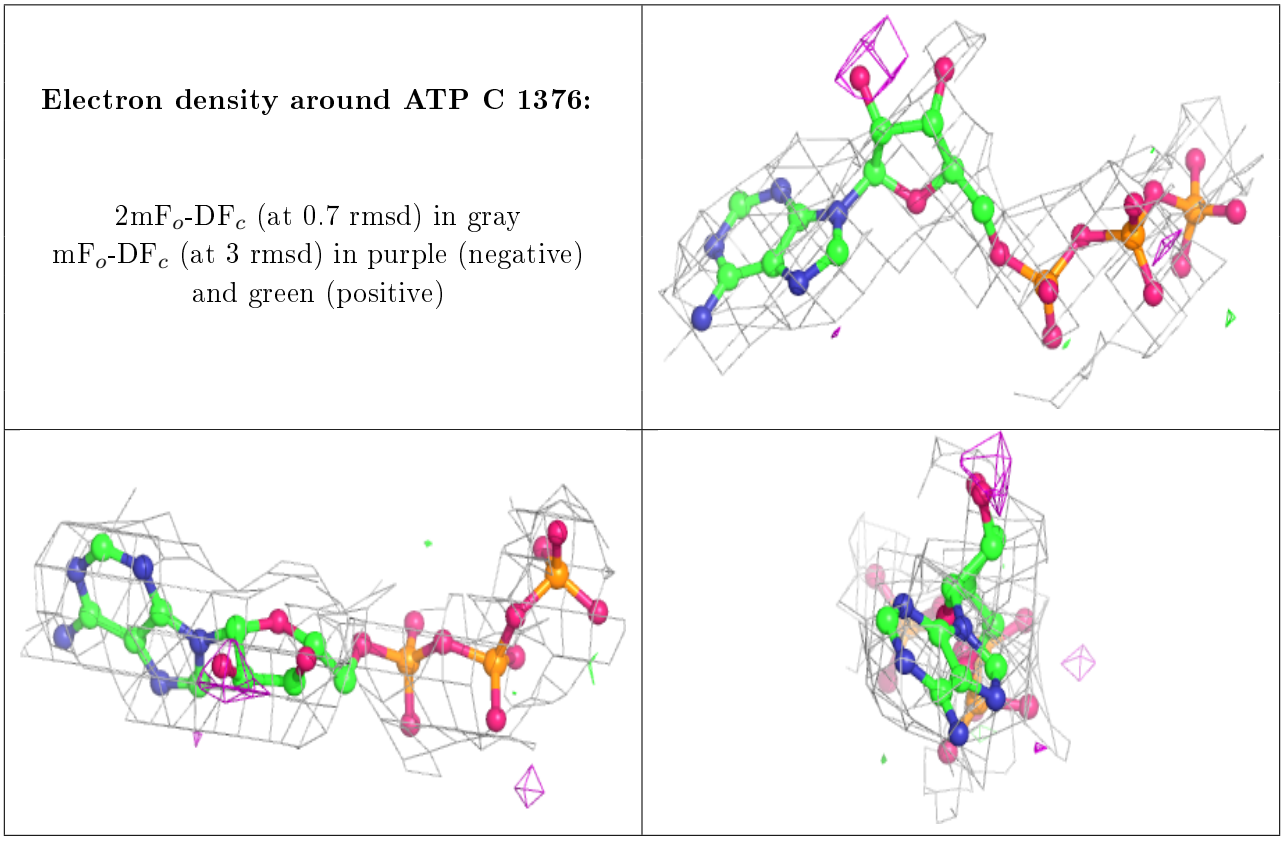
6.4 Ligands

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.

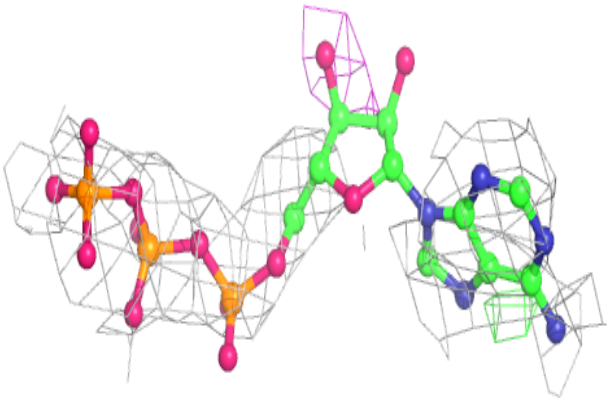
Electron density around ATP C 1376:

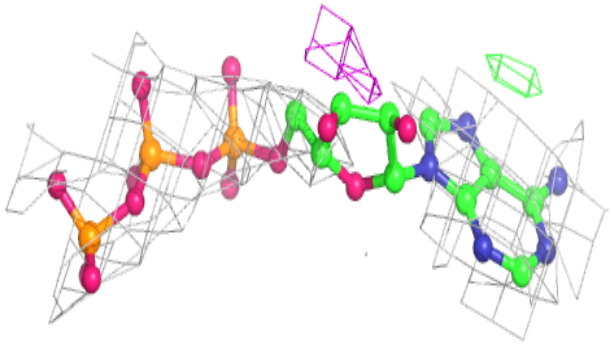
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

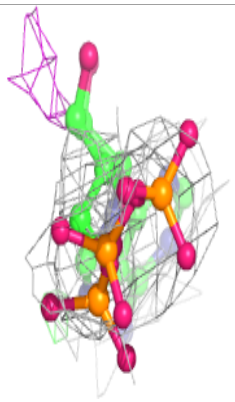


Electron density around ATP A 1376:

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

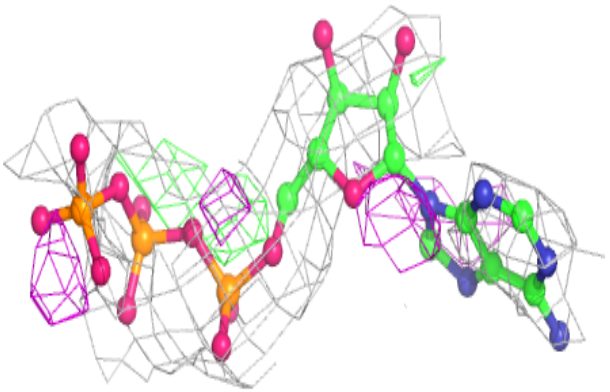


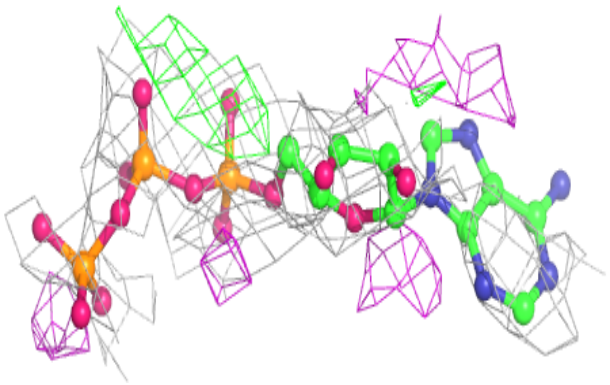


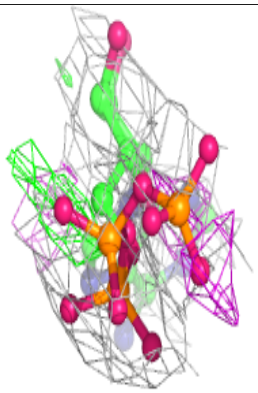


Electron density around ATP B 1376:

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

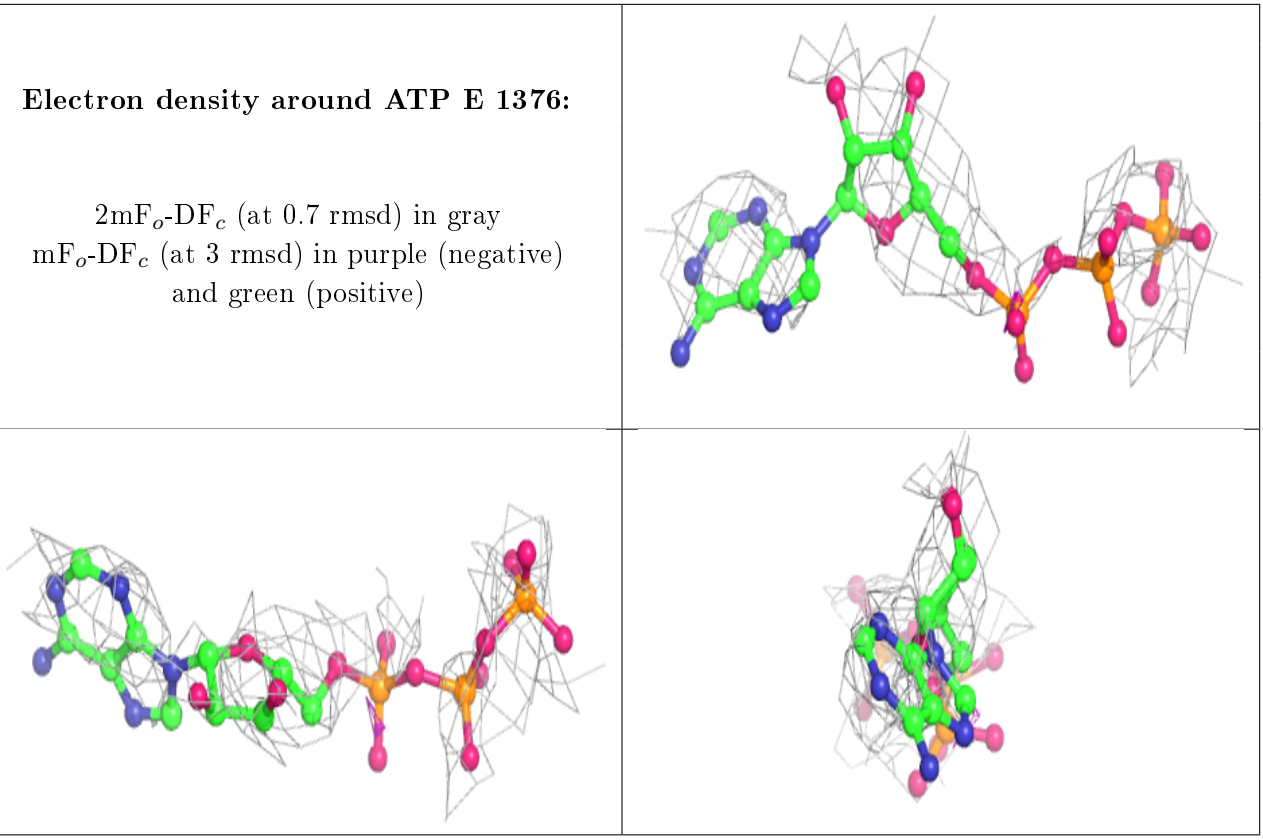






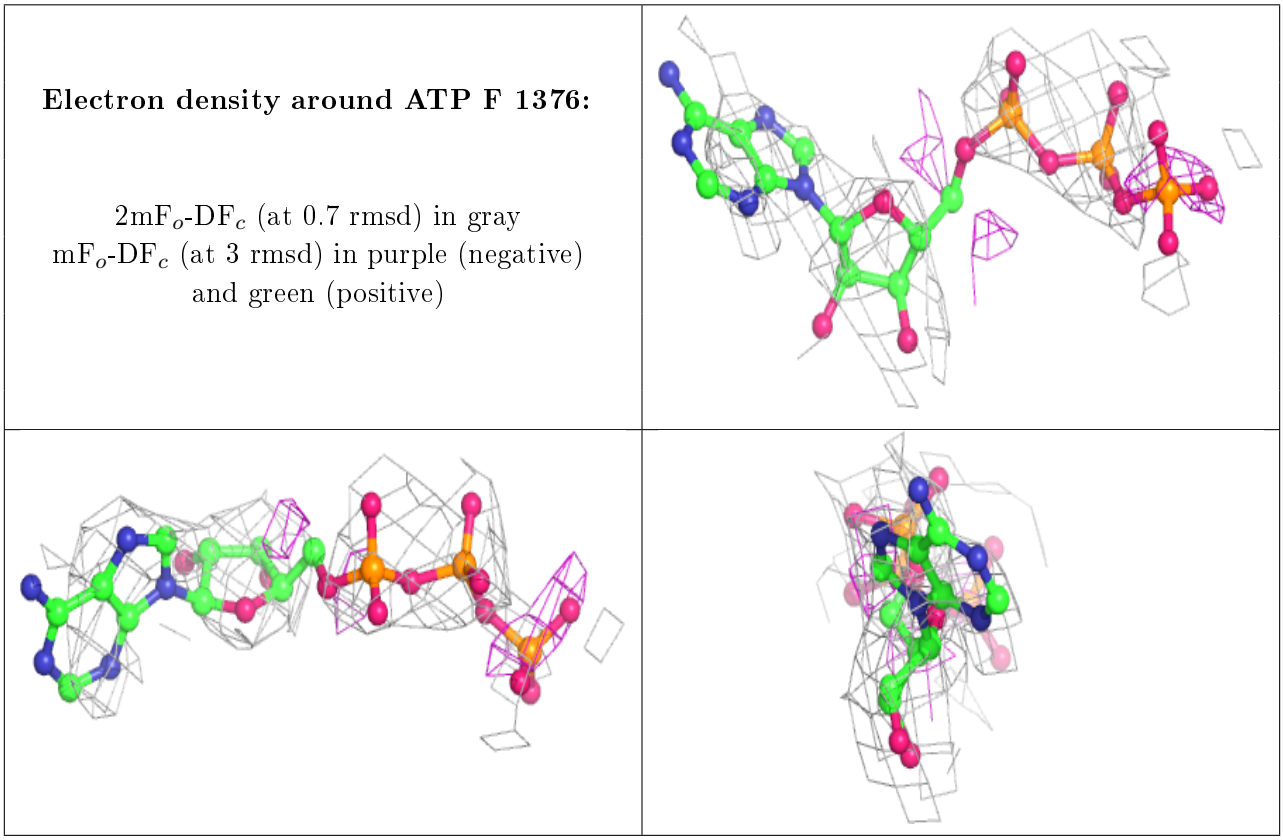
Electron density around ATP E 1376:

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



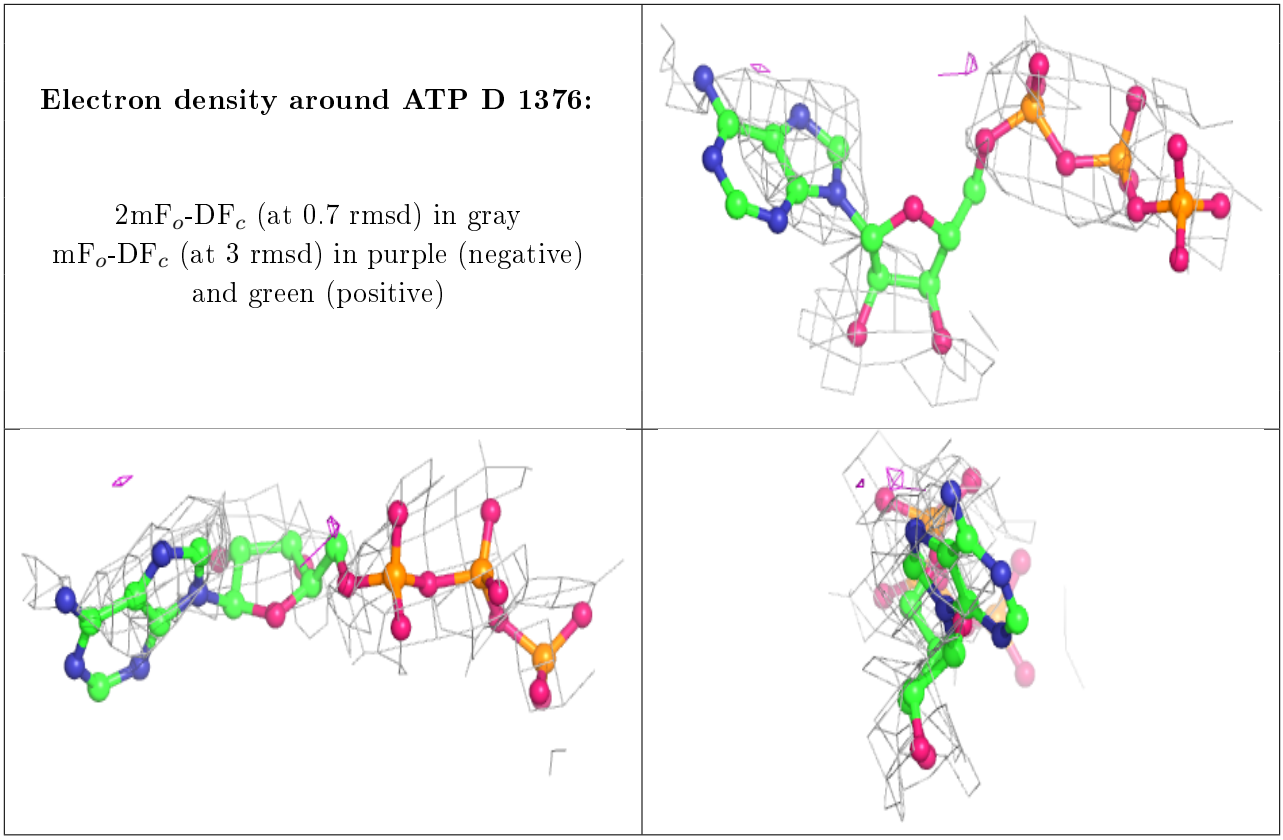
Electron density around ATP F 1376:

$2mF_o$-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 D 1376:

$2mF_o$-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.