wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2024 – 09:54 am GMT

PDB ID	:	6FL3
Title	:	Inositol 1,3,4,5,6-pentakisphosphate 2-kinase from A. thaliana in complex with myo-IP5 and ADP
Authors	:	Whitfield, H.L.; Brearley, C.A.; Hemmings, A.M.
Deposited on	:	2018-01-25
Resolution	:	2.36 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

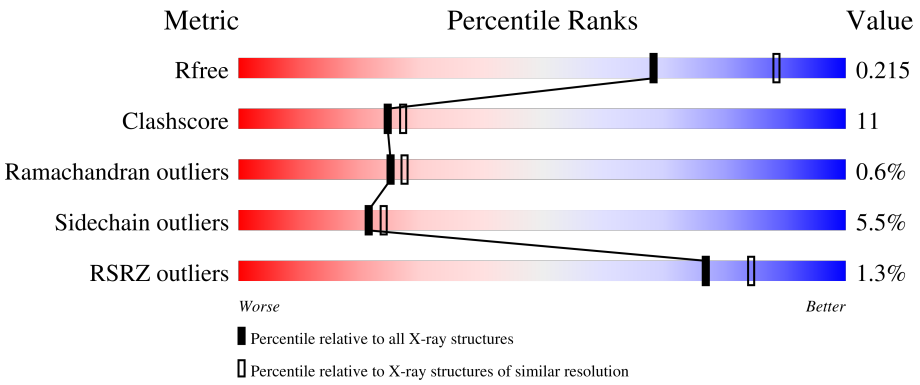
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	470	2% 69% 19% • 10%
1	B	470	% 69% 18% • 11%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7357 atoms, of which 66 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 Inositol-pentakisphosphate 2-kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3371	2145	570	642	14	0	0	0
1	B	420	3344	2128	567	635	14	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A0A178UAB5
A	-17	ALA	-	expression tag	UNP A0A178UAB5
A	-16	HIS	-	expression tag	UNP A0A178UAB5
A	-15	HIS	-	expression tag	UNP A0A178UAB5
A	-14	HIS	-	expression tag	UNP A0A178UAB5
A	-13	HIS	-	expression tag	UNP A0A178UAB5
A	-12	HIS	-	expression tag	UNP A0A178UAB5
A	-11	HIS	-	expression tag	UNP A0A178UAB5
A	-10	SER	-	expression tag	UNP A0A178UAB5
A	-9	SER	-	expression tag	UNP A0A178UAB5
A	-8	GLY	-	expression tag	UNP A0A178UAB5
A	-7	LEU	-	expression tag	UNP A0A178UAB5
A	-6	GLU	-	expression tag	UNP A0A178UAB5
A	-5	VAL	-	expression tag	UNP A0A178UAB5
A	-4	LEU	-	expression tag	UNP A0A178UAB5
A	-3	PHE	-	expression tag	UNP A0A178UAB5
A	-2	GLN	-	expression tag	UNP A0A178UAB5
A	-1	GLY	-	expression tag	UNP A0A178UAB5
A	0	PRO	-	expression tag	UNP A0A178UAB5
A	185	MET	ILE	conflict	UNP A0A178UAB5
B	-18	MET	-	initiating methionine	UNP A0A178UAB5
B	-17	ALA	-	expression tag	UNP A0A178UAB5
B	-16	HIS	-	expression tag	UNP A0A178UAB5
B	-15	HIS	-	expression tag	UNP A0A178UAB5
B	-14	HIS	-	expression tag	UNP A0A178UAB5

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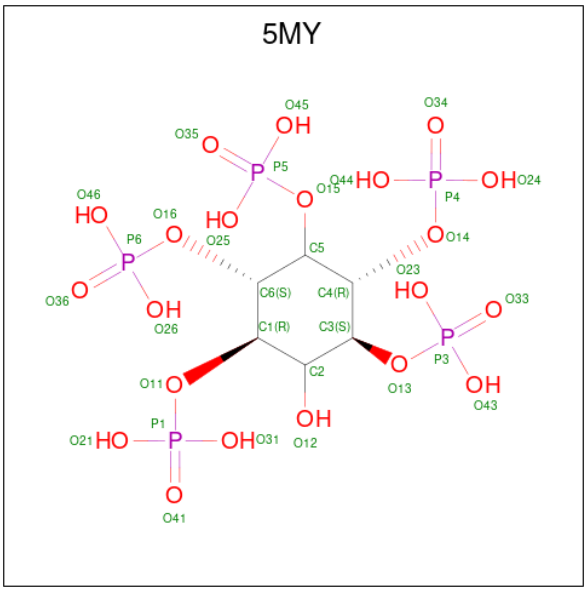
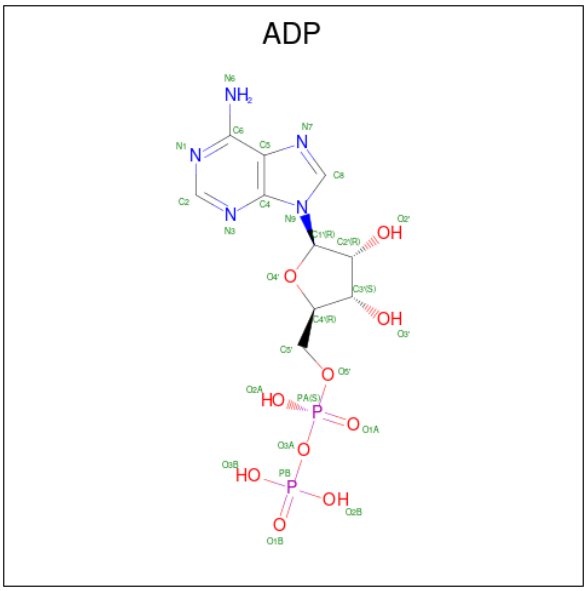
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP A0A178UAB5
B	-12	HIS	-	expression tag	UNP A0A178UAB5
B	-11	HIS	-	expression tag	UNP A0A178UAB5
B	-10	SER	-	expression tag	UNP A0A178UAB5
B	-9	SER	-	expression tag	UNP A0A178UAB5
B	-8	GLY	-	expression tag	UNP A0A178UAB5
B	-7	LEU	-	expression tag	UNP A0A178UAB5
B	-6	GLU	-	expression tag	UNP A0A178UAB5
B	-5	VAL	-	expression tag	UNP A0A178UAB5
B	-4	LEU	-	expression tag	UNP A0A178UAB5
B	-3	PHE	-	expression tag	UNP A0A178UAB5
B	-2	GLN	-	expression tag	UNP A0A178UAB5
B	-1	GLY	-	expression tag	UNP A0A178UAB5
B	0	PRO	-	expression tag	UNP A0A178UAB5
B	185	MET	ILE	conflict	UNP A0A178UAB5

- Molecule 2 is MYO-INOSITOL-(1,3,4,5,6)-PENTAKISPHOSPHATE (three-letter code: 5MY) (formula: $C_6H_{17}O_{21}P_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			39	6	7	21	5		
2	B	1	Total	C	H	O	P	0	0
			39	6	7	21	5		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

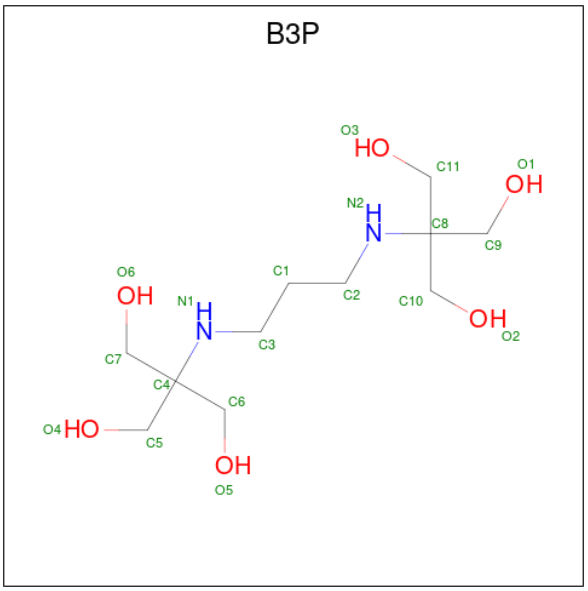
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
6	A	1	45	11	26	2	6	0	0
			Total	C	H	N	O		
6	B	1	45	11	26	2	6	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	202	202	202	0	0
			Total	O		
7	B	212	212	212	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: Inositol-pentakisphosphate 2-kinase

Chain A: 2% 69% 19% • 10%

MET ALA HIS HIS HIS HIS HIS SER SER GLY LEU E-6 E7 L25 S31 V35 G36 I39 R45 R46 ASN ASP K49 A50 I51 K52 V57 V60 Q66 E71 P79 V83 L84 R87 I93 K100 H101 E113 E116 C117 V118 D119

K120 K121 K124 Q125 L128 A133 V136 D148 H149 S150 L151 Q154 GLY ILE THR S158 V165 K168 G172 F179 E183 N184 M185 S189 K194 Q197 L198 E202 S207 E208 F218 V225 I229 N239 V242 G246 E263

Y266 E269 G274 F275 I276 Q277 S278 E279 H282 R283 L290 V295 Y296 K312 Y323 D324 I325 P331 K334 GLU GLY ARG PRO LEU E340 A341 E342 L343 S344 L345 H346 L354 K355 K358 E359 S370 S374 S377 R378 ASN ALA TRP ASP SER GLU

PRO SER GLY D388 Y389 V390 S391 L392 K393 P394 T395 N396 Q397 T398 Y401 K402 I406 D407 L408 S409 L410 K411 K414 S418 K424 S428 R432 K433 Q434 E437 ASN THR ALA GLU GLN ILE GLY ASN SER LYS PRO SER HIS SER

• Molecule 1: Inositol-pentakisphosphate 2-kinase

Chain B: % 69% 18% • 11%

MET ALA HIS HIS HIS HIS HIS SER SER GLY LEU E-6 V-5 I4 L5 E6 E7 K8 D12 W13 I14 Y15 E18 L25 A26 Y27 K37 K43 A44 R45 R46 ASN ASP LYS ALA ILE LYS ASN SER ASN GLY VAL VAL S59 E74 P79 V83 R87 Y88

V89 Q90 N91 V92 I93 I94 G105 V110 E113 V118 K124 D137 L144 D148 H149 S150 S153 Q154 GLY ILE THR SER G159 I163 I167 K168 P169 G172 S177 R178 F179 I180 G181 K182 E183 N184 M185 S207 E208 L215 D216 L217 F218 S219 G220

S221 F243 S247 S256 T260 I264 F268 E269 L272 K273 G274 F275 R283 L290 V300 L301 H320 I325 P329 C330 P331 I332 C333 K334 E335 G336 R337 PRO LEU GLU ALA E342 L343 S344 L345 H346 S370 S374 S377 R378 N379 A380 W381 D382

SER GLU PRO S386 V390 S391 L392 T395 N396 Q397 T398 Y401 K402 V403 I406 D407 L408 Q434 K435 A436 GLU ASN THR ALA GLU GLN ILE GLY ASN SER LYS PRO SER HIS SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.95Å 59.01Å 83.36Å 88.98° 89.56° 63.65°	Depositor
Resolution (Å)	52.87 – 2.36 52.87 – 2.36	Depositor EDS
% Data completeness (in resolution range)	91.8 (52.87-2.36) 91.8 (52.87-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.154 , 0.217 0.155 , 0.215	Depositor DCC
R_{free} test set	1898 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l 0.019 for k,h,-l 0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7357	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: B3P, ZN, ADP, 5MY, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.38	0/3430	0.55	0/4620
1	B	0.41	0/3405	0.54	0/4586
All	All	0.40	0/6835	0.55	0/9206

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 (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	3371	0	3392	72	0
1	B	3344	0	3356	77	0
2	A	32	7	7	1	0
2	B	32	7	7	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	19	26	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	19	26	26	1	0
7	A	202	0	0	4	0
7	B	212	0	0	5	0
All	All	7291	66	6838	149	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 11.

The worst 5 of 149 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:93:ILE:HG21	1:A:408:LEU:HD13	1.45	0.98
1:B:74:GLU:HG3	1:B:91:ASN:ND2	1.92	0.83
1:A:165:VAL:HG22	1:A:242:VAL:HG22	1.65	0.78
1:B:74:GLU:N	1:B:74:GLU:OE1	2.16	0.77
1:B:407:ASP:OD1	7:B:601:HOH:O	2.04	0.75

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	415/470 (88%)	398 (96%)	13 (3%)	4 (1%)	15 15
1	B	410/470 (87%)	393 (96%)	16 (4%)	1 (0%)	47 56
All	All	825/940 (88%)	791 (96%)	29 (4%)	5 (1%)	25 27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	GLU

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Mol	Chain	Res	Type
1	A	343	LEU
1	A	344	SER
1	A	394	PRO
1	B	336	GLY

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	377/415 (91%)	356 (94%)	21 (6%)	21 23
1	B	373/415 (90%)	353 (95%)	20 (5%)	22 25
All	All	750/830 (90%)	709 (94%)	41 (6%)	21 24

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	207	SER
1	B	334	LYS
1	B	208	GLU
1	B	256	SER
1	B	377	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	GLN
1	B	91	ASN
1	B	154	GLN
1	B	289	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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
6	B3P	B	506	-	18,18,18	0.75	0	21,23,23	1.16	3 (14%)
2	5MY	A	501	-	32,32,32	0.69	0	48,53,53	1.18	2 (4%)
2	5MY	B	501	4	32,32,32	0.74	0	48,53,53	1.29	7 (14%)
3	ADP	B	502	4	24,29,29	0.95	1 (4%)	29,45,45	1.43	4 (13%)
3	ADP	A	502	4	24,29,29	1.14	3 (12%)	29,45,45	1.11	3 (10%)
6	B3P	A	506	-	18,18,18	0.47	0	21,23,23	1.08	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	B3P	B	506	-	-	11/28/28/28	-
2	5MY	A	501	-	-	3/25/49/49	0/1/1/1
2	5MY	B	501	4	-	9/25/49/49	0/1/1/1
3	ADP	B	502	4	-	1/12/32/32	0/3/3/3
3	ADP	A	502	4	-	1/12/32/32	0/3/3/3
6	B3P	A	506	-	-	8/28/28/28	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ADP	C5-C4	2.66	1.48	1.40
3	B	502	ADP	C5-C4	2.47	1.47	1.40
3	A	502	ADP	C2-N3	2.41	1.36	1.32
3	A	502	ADP	O4'-C1'	2.28	1.44	1.41

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	5MY	O16-C6-C1	-3.48	100.49	108.69
3	B	502	ADP	PA-O3A-PB	-2.97	122.63	132.83
3	B	502	ADP	N3-C2-N1	-2.87	124.19	128.68
6	B	506	B3P	O5-C6-C4	-2.83	105.91	111.63
3	B	502	ADP	C4-C5-N7	-2.80	106.48	109.40

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	5MY	C3-O13-P3-O33
2	B	501	5MY	C1-O11-P1-O41
6	A	506	B3P	C1-C2-N2-C8
6	A	506	B3P	C9-C8-N2-C2
6	A	506	B3P	C10-C8-N2-C2

There are no ring outliers.

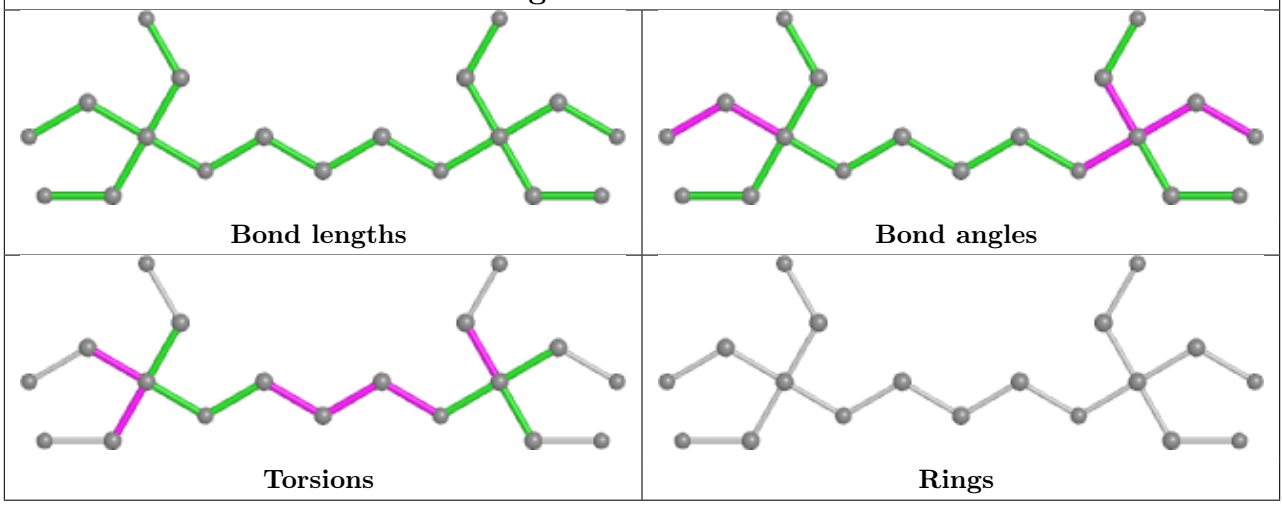
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	506	B3P	1	0
2	A	501	5MY	1	0
3	B	502	ADP	1	0

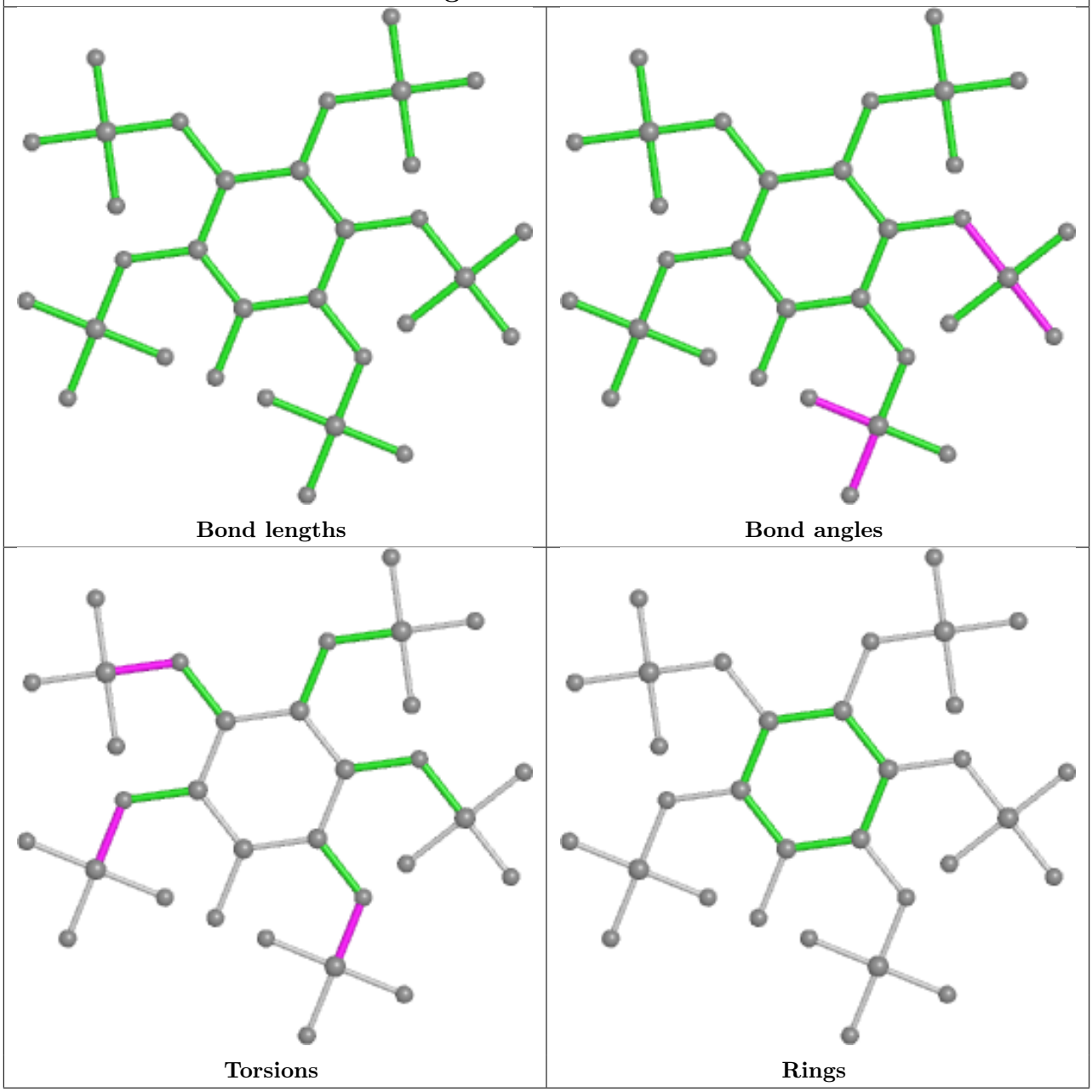
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

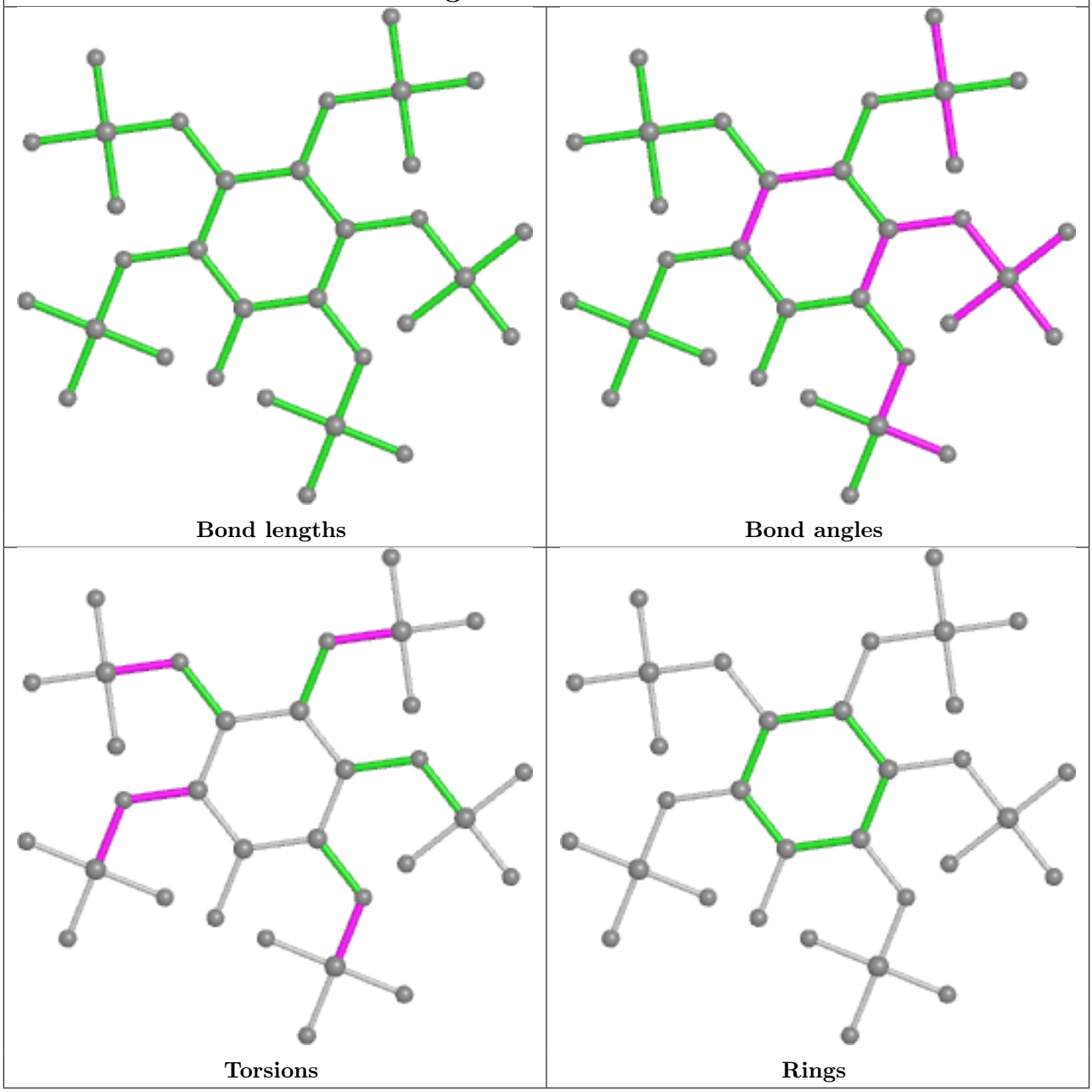
Ligand B3P B 506



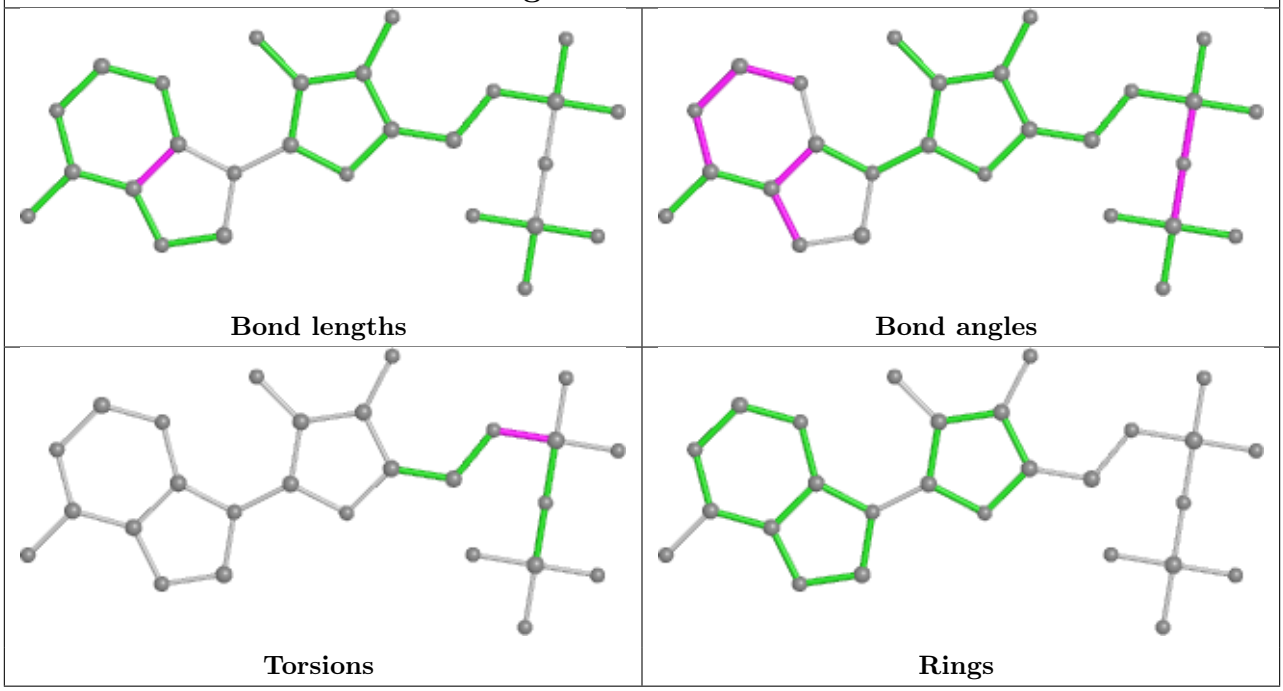
Ligand 5MY A 501



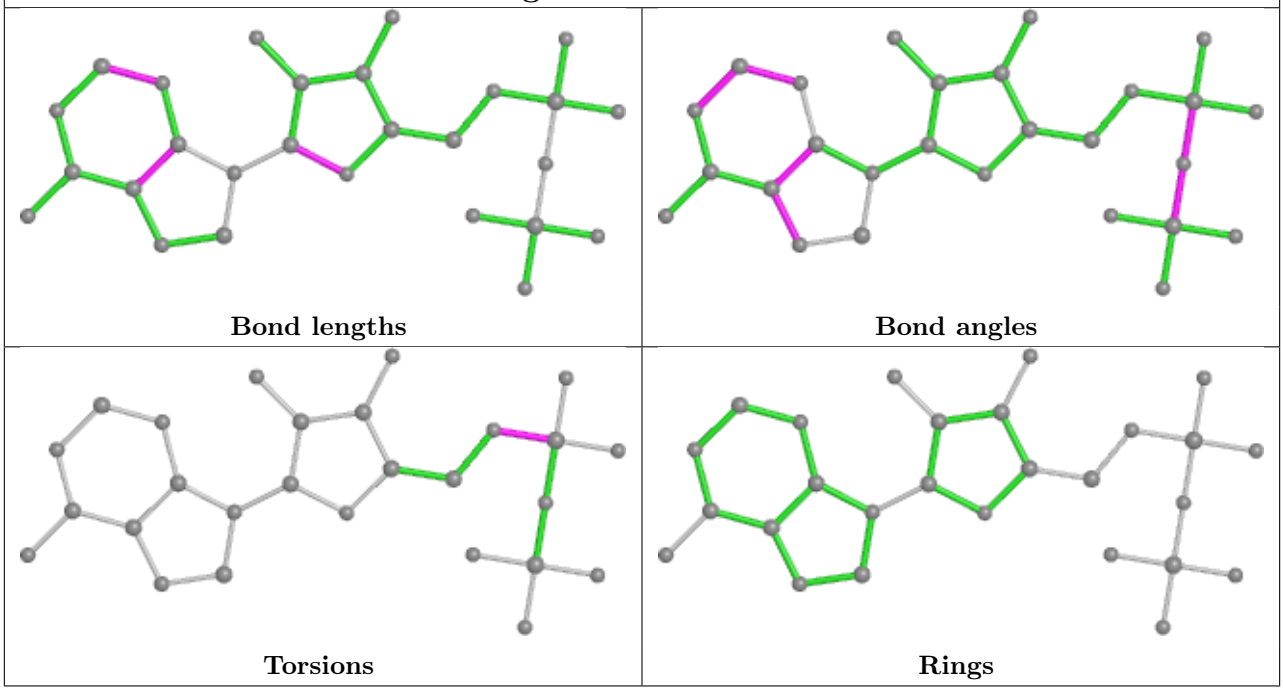
Ligand 5MY B 501

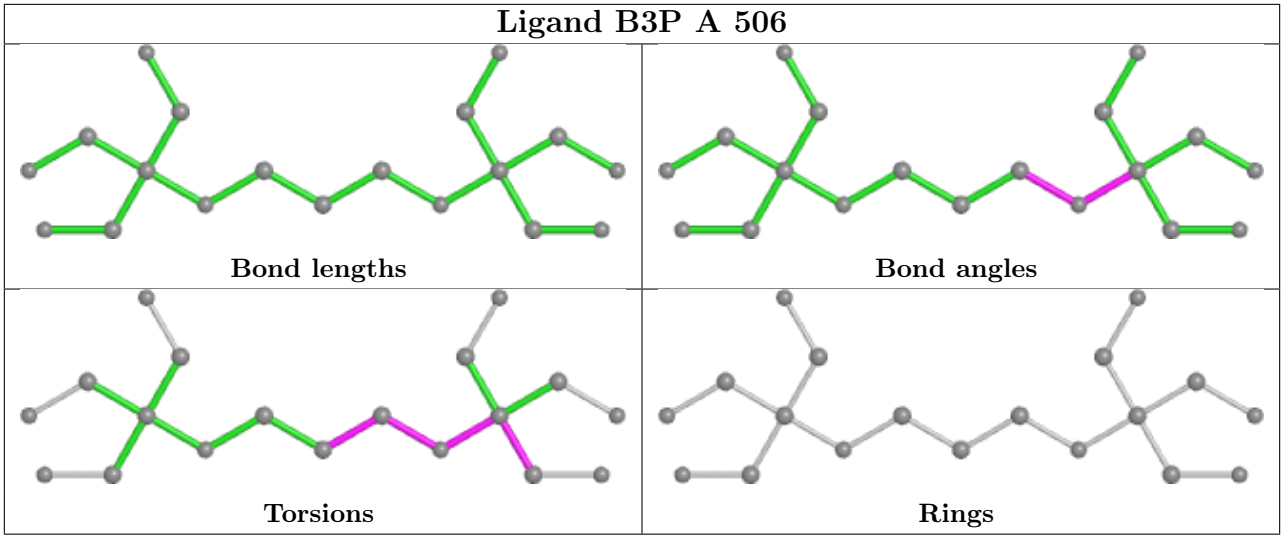


Ligand ADP B 502



Ligand ADP A 502





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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	425/470 (90%)	-0.08	8 (1%)	66	76	15, 35, 76, 115	0
1	B	420/470 (89%)	-0.11	3 (0%)	87	92	15, 34, 66, 133	0
All	All	845/940 (89%)	-0.10	11 (1%)	77	84	15, 35, 74, 133	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	GLN	5.4
1	A	378	ARG	5.4
1	A	276	ILE	4.0
1	A	391	SER	2.8
1	B	335	GLU	2.7

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)

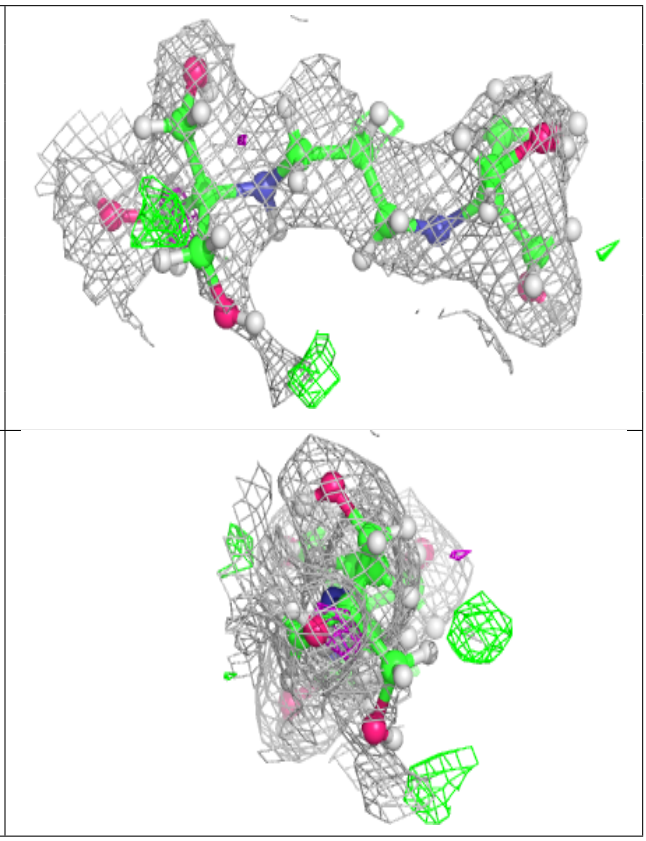
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B3P	A	506	19/19	0.86	0.16	40,62,89,92	0
4	MG	A	504	1/1	0.92	0.11	24,24,24,24	0
4	MG	B	504	1/1	0.93	0.14	24,24,24,24	0
6	B3P	B	506	19/19	0.94	0.15	20,47,84,94	0
4	MG	A	503	1/1	0.97	0.23	24,24,24,24	0
4	MG	B	503	1/1	0.98	0.11	27,27,27,27	0
3	ADP	B	502	27/27	0.98	0.12	17,24,28,31	0
2	5MY	A	501	32/32	0.98	0.13	17,26,37,38	0
3	ADP	A	502	27/27	0.98	0.11	15,22,26,28	0
2	5MY	B	501	32/32	0.99	0.12	14,26,35,38	0
5	ZN	A	505	1/1	1.00	0.14	29,29,29,29	0
5	ZN	B	505	1/1	1.00	0.13	27,27,27,27	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.

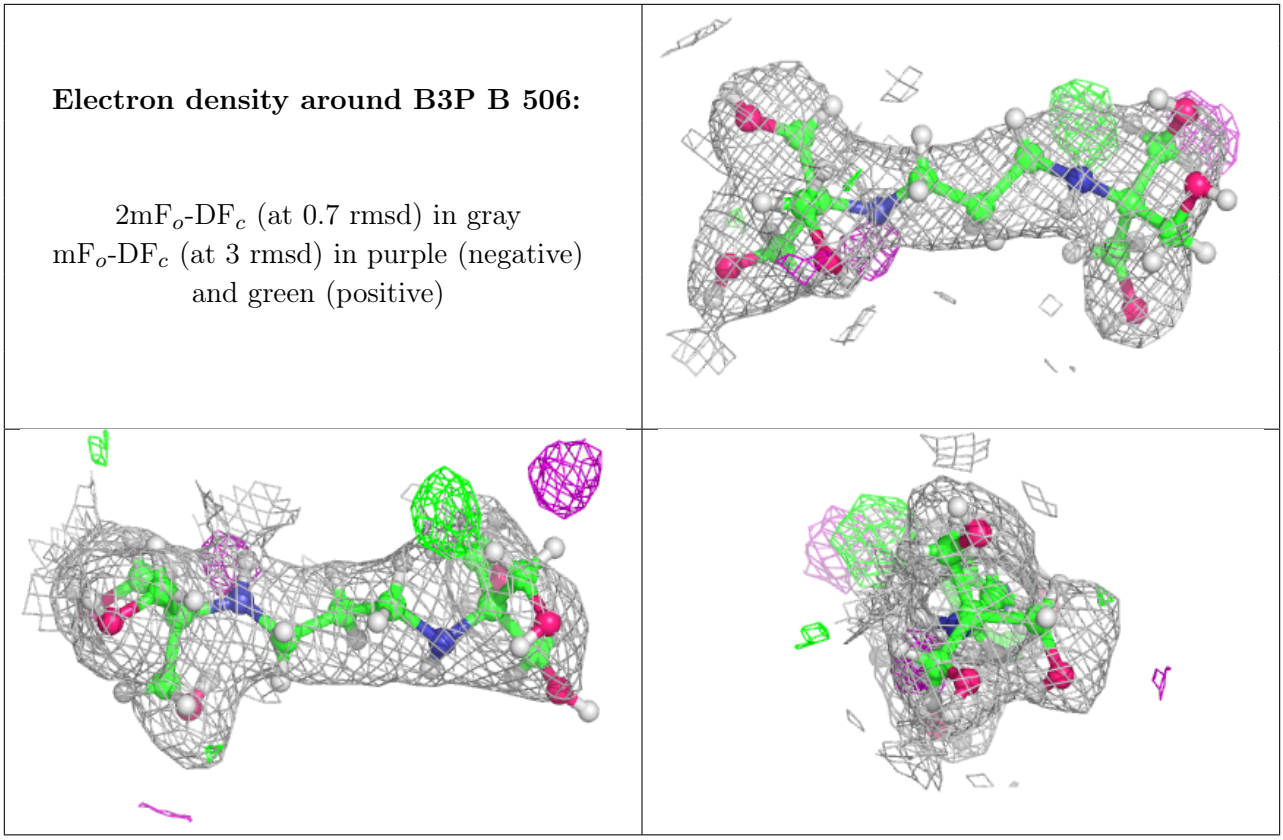
Electron density around B3P A 506:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



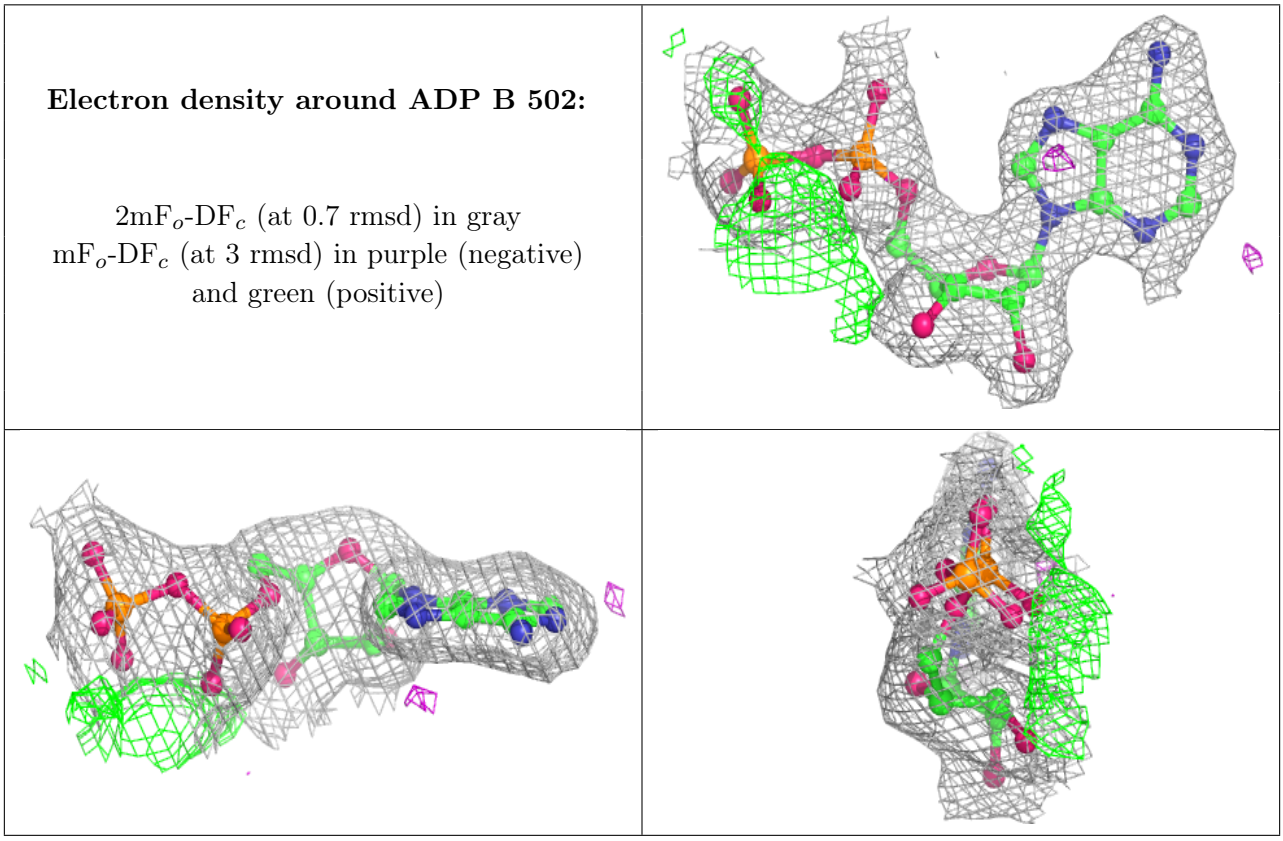
Electron density around B3P B 506:

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



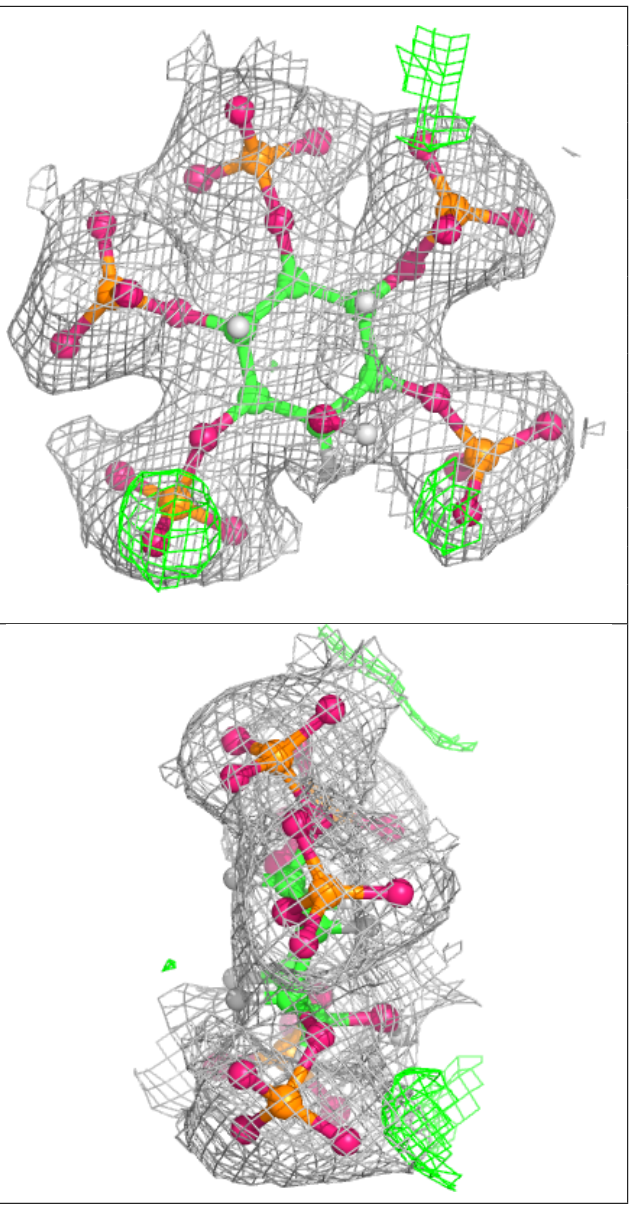
Electron density around ADP B 502:

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



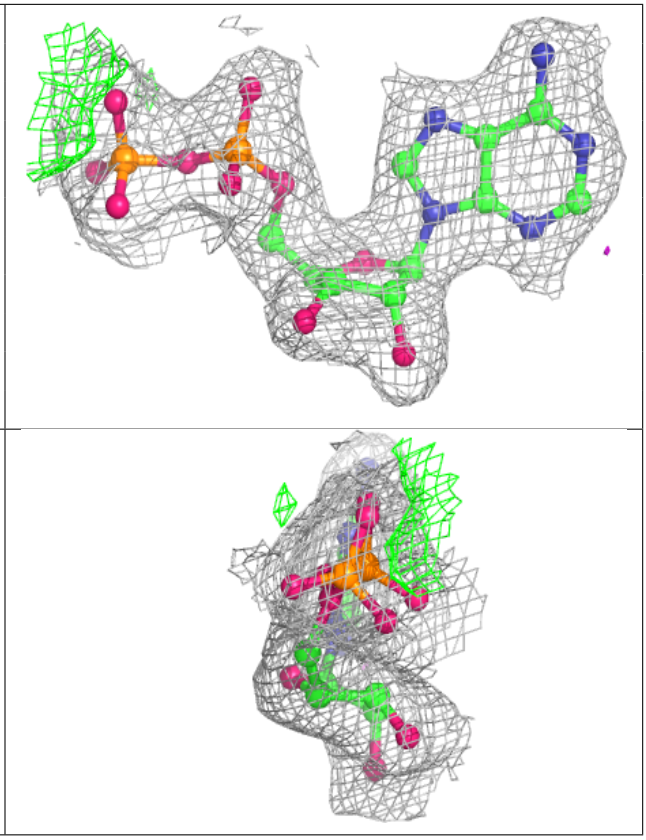
Electron density around 5MY A 501:

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



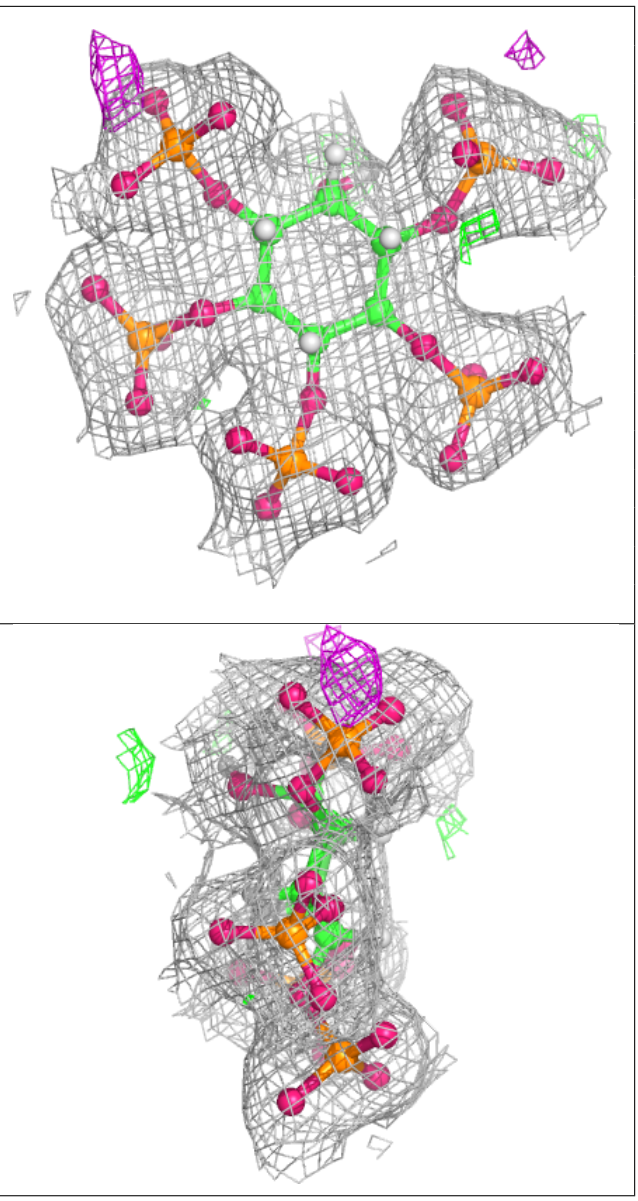
Electron density around ADP A 502:

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



Electron density around 5MY B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.