Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 01:00 AM EDT

PDB ID	:	5KOY
Title	:	Mouse pgp 34 linker deleted bound with ATP
Authors	:	Xia, D.; Esser, L.; Zhou, F.
Deposited on	:	2016-07-01
Resolution	:	3.85 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:

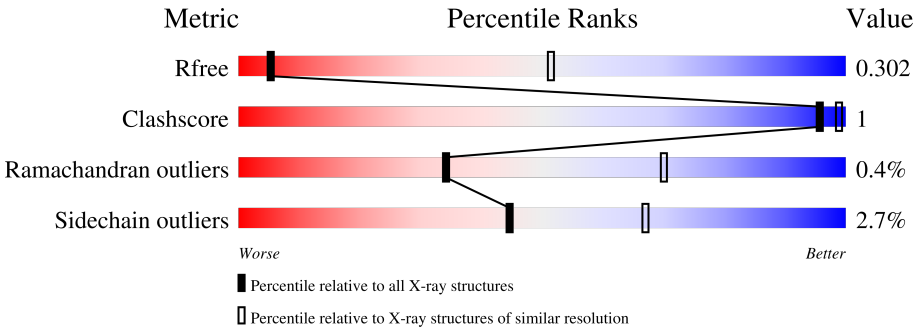
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.85 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	1048 (4.10-3.62)
Clashscore	141614	1015 (4.08-3.64)
Ramachandran outliers	138981	1069 (4.10-3.62)
Sidechain outliers	138945	1062 (4.10-3.62)

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	1248	90% 5% 5%
1	B	1248	88% 6% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 37055 atoms, of which 18673 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 Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1182	Total	C	H	N	O	S	0	0	0
			18488	5890	9326	1554	1680	38			
1	B	1181	Total	C	H	N	O	S	0	0	0
			18481	5888	9323	1553	1679	38			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	GLN	GLU	engineered mutation	UNP P21447
A	?	-	MET	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	ASP	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	GLY	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	LEU	deletion	UNP P21447
A	?	-	ILE	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	THR	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	ILE	deletion	UNP P21447
A	?	-	CYS	deletion	UNP P21447
A	?	-	GLY	deletion	UNP P21447
A	?	-	PRO	deletion	UNP P21447
A	?	-	HIS	deletion	UNP P21447

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P21447
A	?	-	GLN	deletion	UNP P21447
A	?	-	ASP	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	LEU	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	THR	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	GLU	deletion	UNP P21447
A	1197	GLN	GLU	conflict	UNP P21447
A	1277	HIS	-	expression tag	UNP P21447
A	1278	HIS	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
B	552	GLN	GLU	engineered mutation	UNP P21447
B	?	-	MET	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	ASP	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	GLY	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	LEU	deletion	UNP P21447
B	?	-	ILE	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	THR	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	ILE	deletion	UNP P21447
B	?	-	CYS	deletion	UNP P21447
B	?	-	GLY	deletion	UNP P21447
B	?	-	PRO	deletion	UNP P21447
B	?	-	HIS	deletion	UNP P21447

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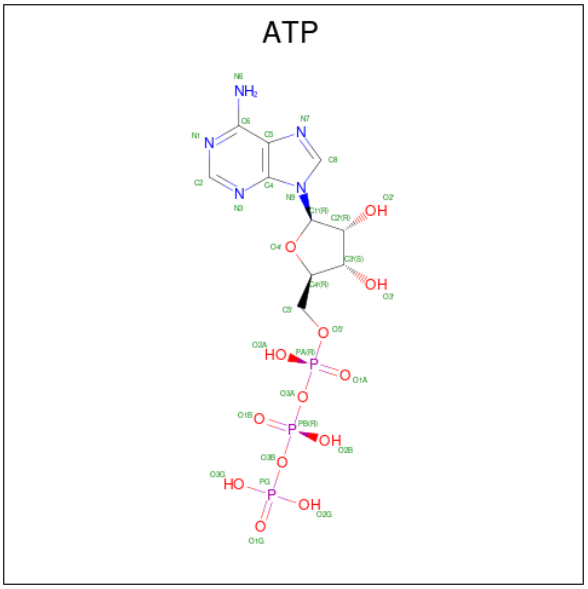
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP P21447
B	?	-	GLN	deletion	UNP P21447
B	?	-	ASP	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	LEU	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	THR	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	GLU	deletion	UNP P21447
B	1197	GLN	GLU	conflict	UNP P21447
B	1277	HIS	-	expression tag	UNP P21447
B	1278	HIS	-	expression tag	UNP P21447
B	1279	HIS	-	expression tag	UNP P21447
B	1280	HIS	-	expression tag	UNP P21447
B	1281	HIS	-	expression tag	UNP P21447
B	1282	HIS	-	expression tag	UNP P21447

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



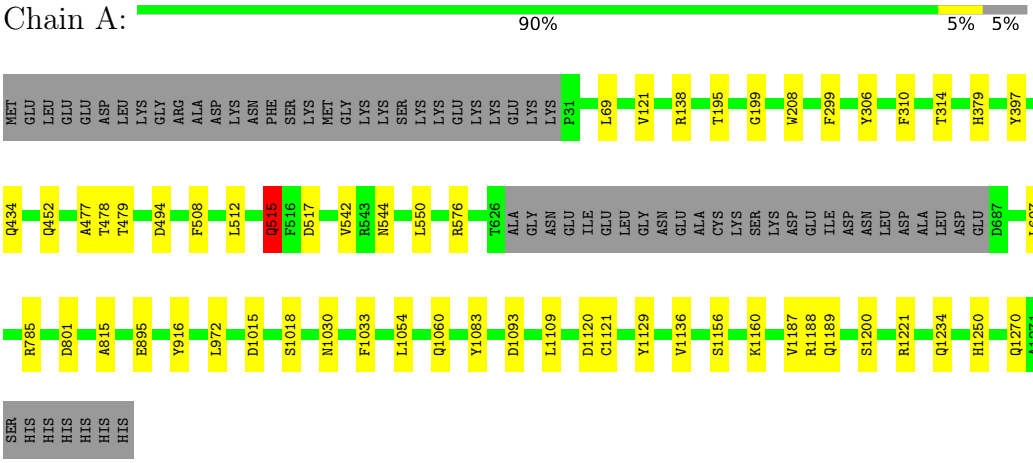
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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.

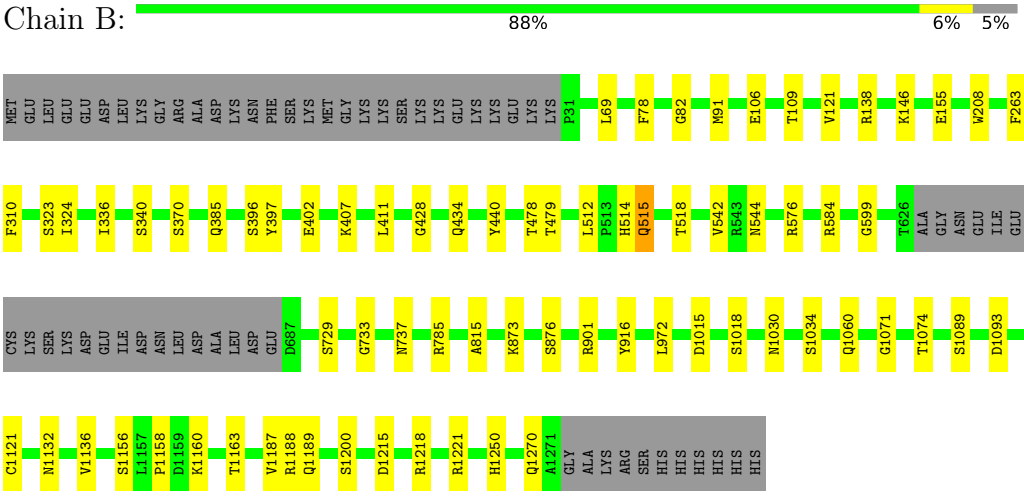
• Molecule 1: Multidrug resistance protein 1A

Chain A:



• Molecule 1: Multidrug resistance protein 1A

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.52Å 116.44Å 375.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.30 – 3.85 49.99 – 3.82	Depositor EDS
% Data completeness (in resolution range)	99.9 (21.30-3.85) 96.6 (49.99-3.82)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.246 , 0.289 0.260 , 0.302	Depositor DCC
R_{free} test set	1996 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	141.5	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 86.3	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	0.84	EDS
Total number of atoms	37055	wwPDB-VP
Average B, all atoms (Å^2)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: 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	0.34	0/9331	0.63	0/12615
1	B	0.33	0/9327	0.62	0/12610
All	All	0.34	0/18658	0.63	0/25225

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	9162	9326	9343	17	0
1	B	9158	9323	9340	27	0
2	A	31	12	12	0	0
2	B	31	12	12	1	0
All	All	18382	18673	18707	41	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 1.

All (41) 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:B:544:ASN:OD1	1:B:576:ARG:NH2	2.24	0.70
1:B:1158:PRO:O	1:B:1163:THR:OG1	2.11	0.69
1:B:397:TYR:OH	1:B:434:GLN:NE2	2.26	0.69
1:A:138:ARG:NH2	1:B:515:GLN:OE1	2.25	0.69
1:B:440:TYR:OH	1:B:901:ARG:NH2	2.26	0.68
1:A:544:ASN:OD1	1:A:576:ARG:NH2	2.28	0.66
1:B:1215:ASP:OD1	1:B:1218:ARG:NH2	2.29	0.65
1:A:1189:GLN:OE1	1:A:1221:ARG:NH2	2.33	0.62
1:B:407:LYS:NZ	1:B:599:GLY:O	2.35	0.60
1:B:428:GLY:N	2:B:2000:ATP:O1A	2.38	0.56
1:A:397:TYR:OH	1:A:434:GLN:NE2	2.39	0.56
1:B:733:GLY:O	1:B:737:ASN:ND2	2.39	0.55
1:A:1109:LEU:O	1:A:1188:ARG:NH1	2.40	0.55
1:A:801:ASP:OD2	1:A:1083:TYR:OH	2.25	0.55
1:B:514:HIS:O	1:B:518:THR:N	2.42	0.52
1:A:515:GLN:OE1	1:B:138:ARG:NH2	2.43	0.51
1:B:1189:GLN:OE1	1:B:1221:ARG:NH2	2.44	0.51
1:B:785:ARG:NH2	1:B:815:ALA:O	2.43	0.49
1:A:1030:ASN:N	1:A:1093:ASP:OD1	2.45	0.49
1:B:155:GLU:OE2	1:B:370:SER:OG	2.29	0.49
1:B:1109:LEU:O	1:B:1188:ARG:NH1	2.45	0.48
1:A:755:PHE:O	1:A:759:GLY:N	2.43	0.48
1:A:379:HIS:ND1	1:A:452:GLN:OE1	2.45	0.48
1:B:1030:ASN:N	1:B:1093:ASP:OD1	2.46	0.47
1:B:1071:GLY:O	1:B:1074:THR:OG1	2.30	0.47
1:A:494:ASP:OD1	1:B:146:LYS:NZ	2.45	0.47
1:A:1033:PHE:O	1:A:1054:LEU:N	2.46	0.46
1:B:1015:ASP:OD2	1:B:1018:SER:N	2.49	0.45
1:A:478:THR:HG22	1:A:479:THR:H	1.82	0.45
1:B:729:SER:O	1:B:733:GLY:N	2.46	0.45
1:B:78:PHE:O	1:B:82:GLY:N	2.49	0.44
1:A:195:THR:O	1:A:199:GLY:N	2.45	0.44
1:B:106:GLU:O	1:B:109:THR:OG1	2.32	0.44
1:B:478:THR:HG22	1:B:479:THR:H	1.82	0.44
1:B:873:LYS:O	1:B:876:SER:N	2.51	0.43
1:A:477:ALA:N	1:A:895:GLU:OE2	2.52	0.43
1:A:1015:ASP:OD1	1:A:1018:SER:N	2.51	0.43
1:A:785:ARG:NH2	1:A:815:ALA:O	2.48	0.42
1:B:263:PHE:O	1:B:1132:ASN:ND2	2.53	0.42
1:B:323:SER:OG	1:B:324:ILE:N	2.53	0.42
1:B:336:ILE:O	1:B:340:SER:N	2.54	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	1178/1248 (94%)	1124 (95%)	49 (4%)	5 (0%)	34	70
1	B	1177/1248 (94%)	1122 (95%)	51 (4%)	4 (0%)	41	74
All	All	2355/2496 (94%)	2246 (95%)	100 (4%)	9 (0%)	34	70

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	GLN
1	A	1136	VAL
1	A	1160	LYS
1	B	515	GLN
1	B	1136	VAL
1	B	1120	ASP
1	A	411	LEU
1	A	1120	ASP
1	B	411	LEU

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	974/1031 (94%)	948 (97%)	26 (3%)	44	67
1	B	974/1031 (94%)	948 (97%)	26 (3%)	44	67
All	All	1948/2062 (94%)	1896 (97%)	52 (3%)	44	67

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	121	VAL
1	A	208	TRP
1	A	299	PHE
1	A	306	TYR
1	A	310	PHE
1	A	314	THR
1	A	402	GLU
1	A	508	PHE
1	A	512	LEU
1	A	515	GLN
1	A	517	ASP
1	A	542	VAL
1	A	550	LEU
1	A	697	LEU
1	A	916	TYR
1	A	972	LEU
1	A	1060	GLN
1	A	1121	CYS
1	A	1129	TYR
1	A	1156	SER
1	A	1187	VAL
1	A	1200	SER
1	A	1234	GLN
1	A	1250	HIS
1	A	1270	GLN
1	B	69	LEU
1	B	91	MET
1	B	121	VAL
1	B	208	TRP
1	B	299	PHE
1	B	306	TYR
1	B	310	PHE
1	B	385	GLN
1	B	396	SER
1	B	402	GLU
1	B	512	LEU
1	B	542	VAL
1	B	584	ARG
1	B	916	TYR
1	B	972	LEU
1	B	1034	SER

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Mol	Chain	Res	Type
1	B	1060	GLN
1	B	1089	SER
1	B	1096	GLU
1	B	1121	CYS
1	B	1156	SER
1	B	1160	LYS
1	B	1187	VAL
1	B	1200	SER
1	B	1250	HIS
1	B	1270	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	GLN
1	A	878	GLN
1	A	926	ASN
1	B	434	GLN
1	B	608	HIS
1	B	910	GLN
1	B	1270	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)

2 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	2000	-	26,33,33	0.93	1 (3%)	31,52,52	1.61	6 (19%)
2	ATP	B	2000	-	26,33,33	0.93	1 (3%)	31,52,52	1.62	6 (19%)

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	2000	-	-	4/18/38/38	0/3/3/3
2	ATP	B	2000	-	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	ATP	C5-C4	2.37	1.47	1.40
2	A	2000	ATP	C5-C4	2.35	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2000	ATP	PA-O3A-PB	-3.95	119.27	132.83
2	A	2000	ATP	PA-O3A-PB	-3.79	119.84	132.83
2	B	2000	ATP	N3-C2-N1	-3.76	122.80	128.68
2	A	2000	ATP	N3-C2-N1	-3.68	122.92	128.68
2	B	2000	ATP	PB-O3B-PG	-3.65	120.31	132.83
2	A	2000	ATP	PB-O3B-PG	-3.46	120.94	132.83
2	A	2000	ATP	C4-C5-N7	-3.11	106.16	109.40
2	B	2000	ATP	C4-C5-N7	-2.88	106.40	109.40
2	A	2000	ATP	C3'-C2'-C1'	2.13	104.19	100.98
2	B	2000	ATP	C2-N1-C6	2.08	122.31	118.75
2	B	2000	ATP	C3'-C2'-C1'	2.03	104.04	100.98
2	A	2000	ATP	C2-N1-C6	2.01	122.20	118.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	ATP	C5'-O5'-PA-O1A
2	A	2000	ATP	C5'-O5'-PA-O3A
2	A	2000	ATP	PG-O3B-PB-O2B
2	B	2000	ATP	C5'-O5'-PA-O2A
2	B	2000	ATP	C5'-O5'-PA-O3A
2	A	2000	ATP	PG-O3B-PB-O1B

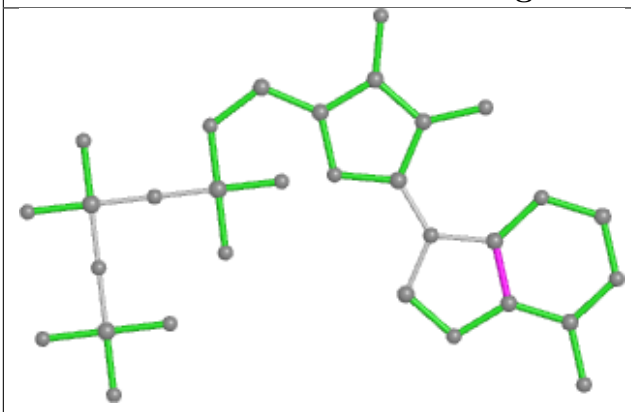
There are no ring outliers.

1 monomer is involved in 1 short contact:

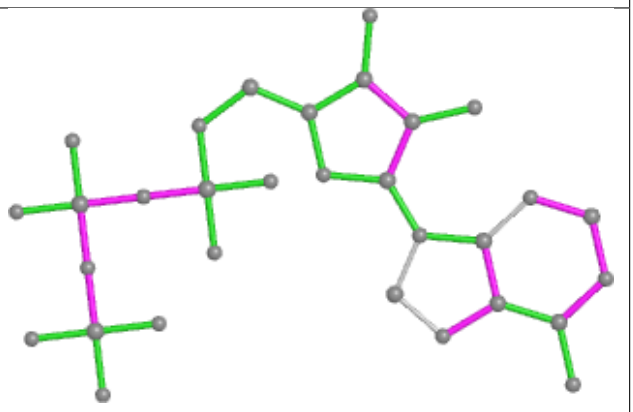
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2000	ATP	1	0

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.

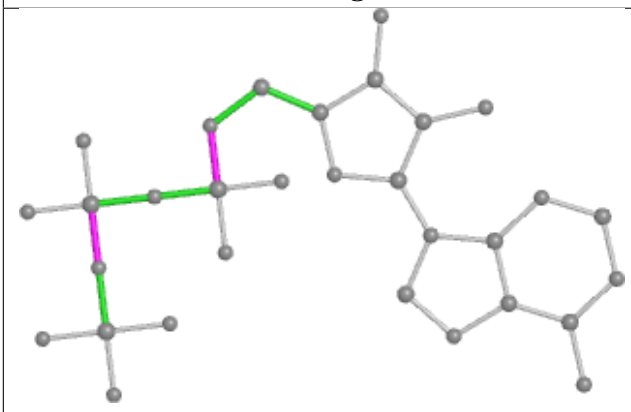
Ligand ATP A 2000



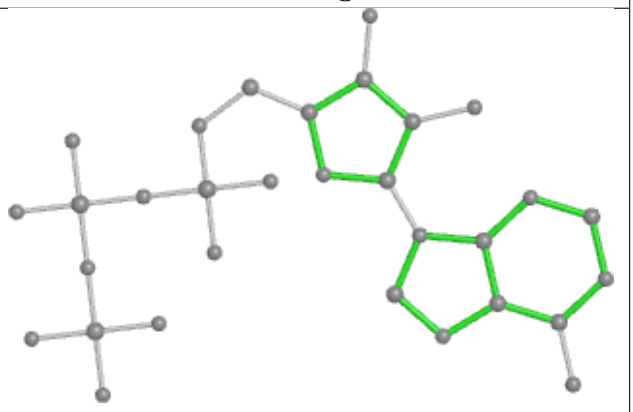
Bond lengths



Bond angles

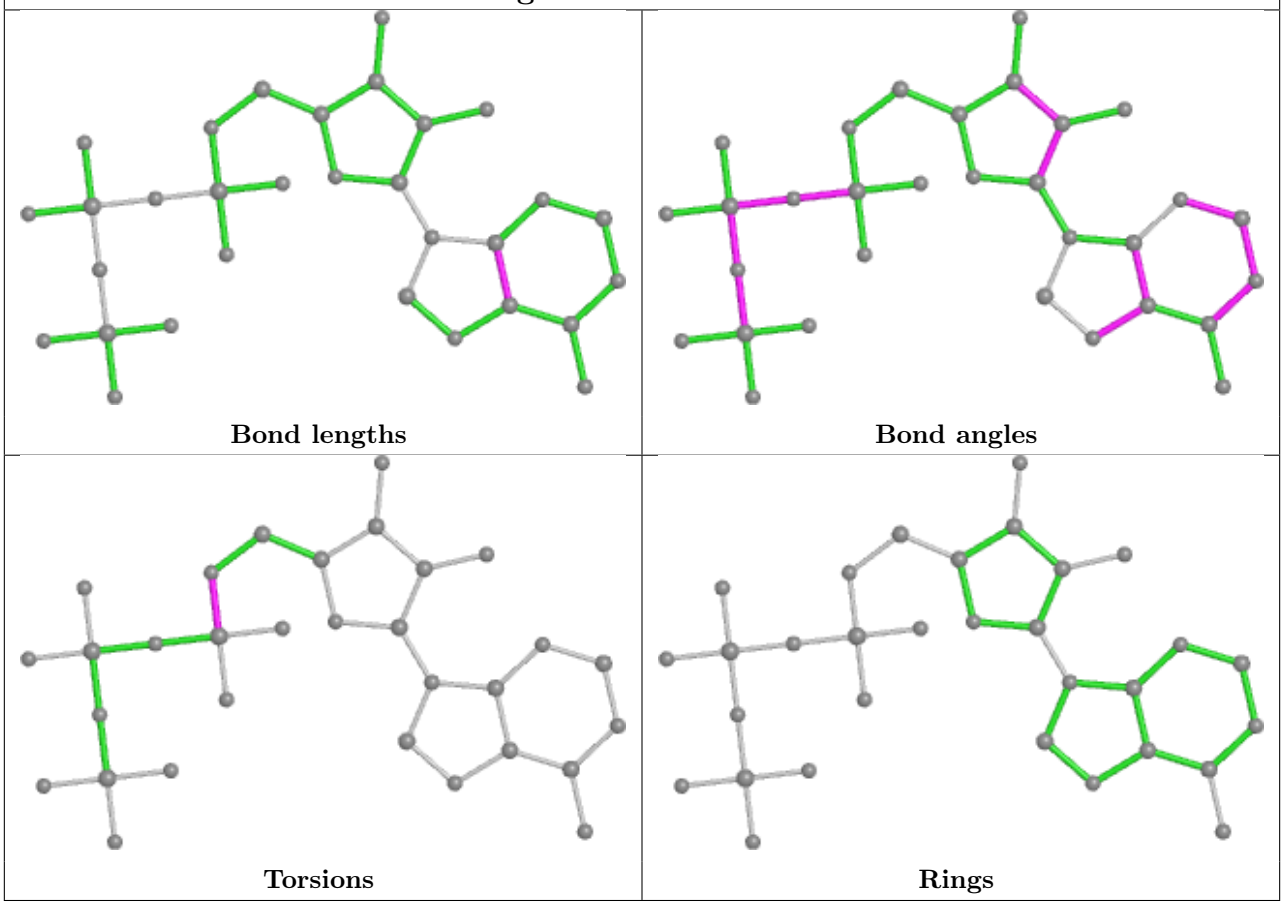


Torsions



Rings

Ligand ATP B 2000



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.

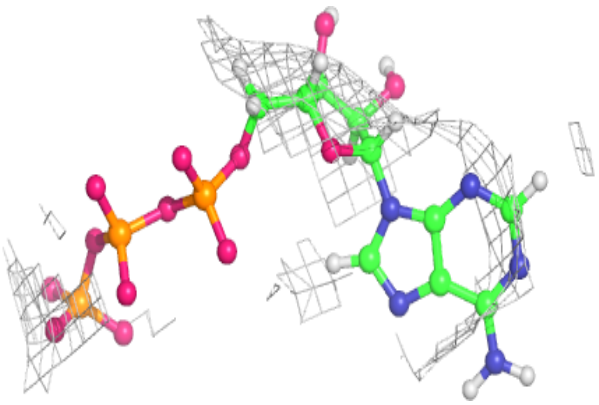
6.4 Ligands

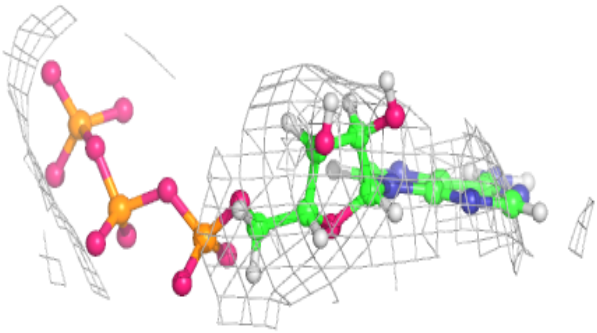
Unable to reproduce the depositors R factor - this section is therefore empty.

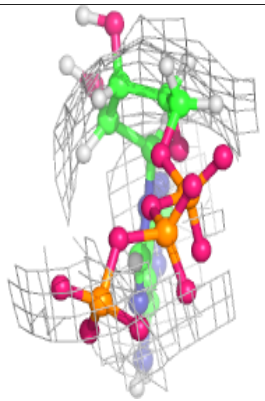
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 2000:

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

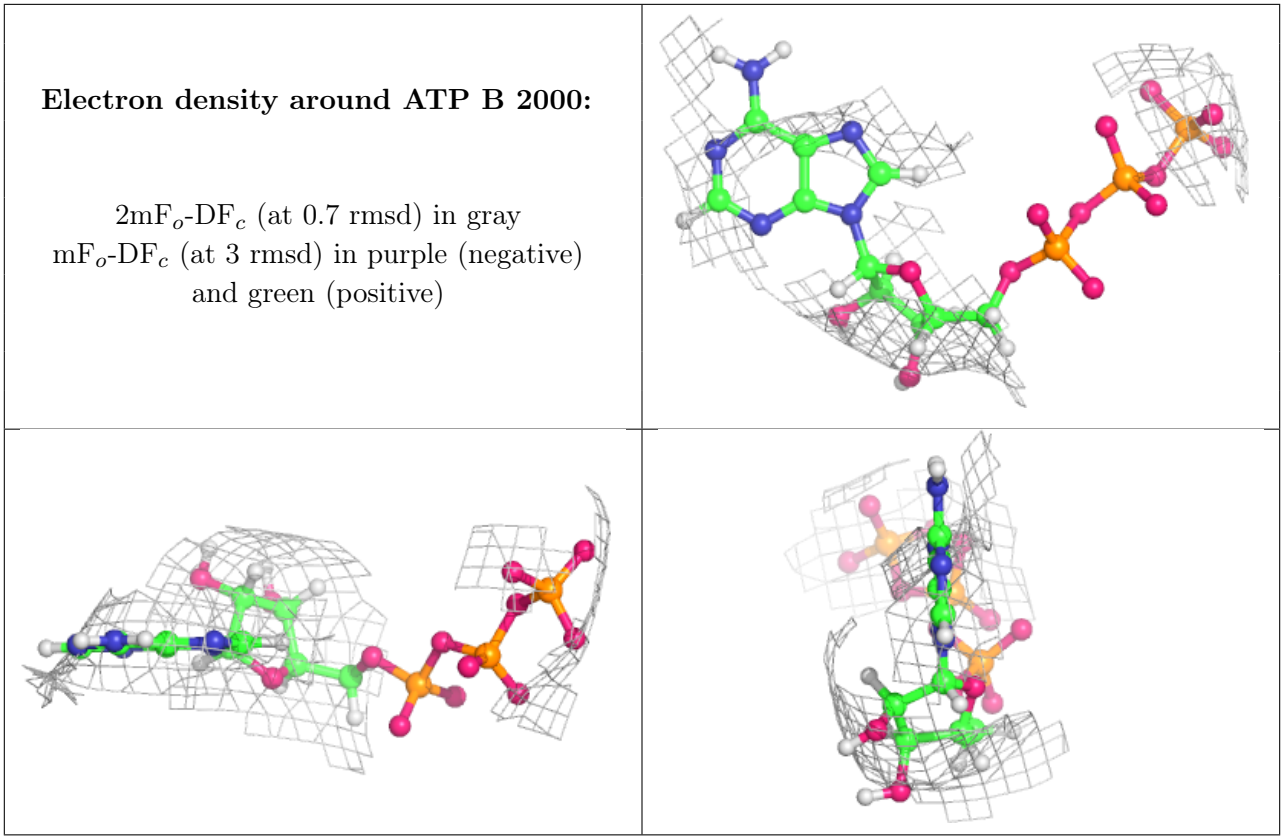






Electron density around ATP B 2000:

$2mF_o$-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.