



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 04:57 pm BST

PDB ID : 13PK
Title : TERNARY COMPLEX OF PHOSPHOGLYCERATE KINASE FROM TRY-
PANOSOMA BRUCEI
Authors : Bernstein, B.E.; Michels, P.A.M.; Hol, W.G.J.
Deposited on : 1996-11-23
Resolution : 2.50 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 ⓘ 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

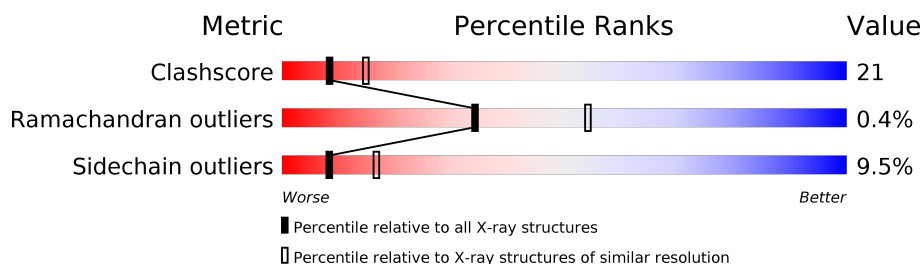
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	415	
1	B	415	
1	C	415	
1	D	415	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	C	624	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	D	625	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13271 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 3-PHOSPHOGLYCERATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3127	1981	542	584	20			
1	B	415	Total	C	N	O	S	0	0	0
			3127	1981	542	584	20			
1	C	415	Total	C	N	O	S	0	0	0
			3127	1981	542	584	20			
1	D	415	Total	C	N	O	S	0	0	0
			3127	1981	542	584	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	ARG	ALA	CONFLICT	UNP P07378
A	418	ASP	GLU	CONFLICT	UNP P07378
B	98	ARG	ALA	CONFLICT	UNP P07378
B	418	ASP	GLU	CONFLICT	UNP P07378
C	98	ARG	ALA	CONFLICT	UNP P07378
C	418	ASP	GLU	CONFLICT	UNP P07378
D	98	ARG	ALA	CONFLICT	UNP P07378
D	418	ASP	GLU	CONFLICT	UNP P07378

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

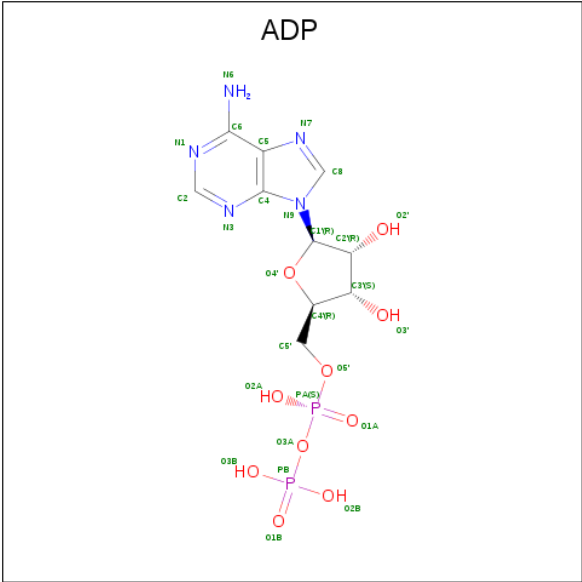
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



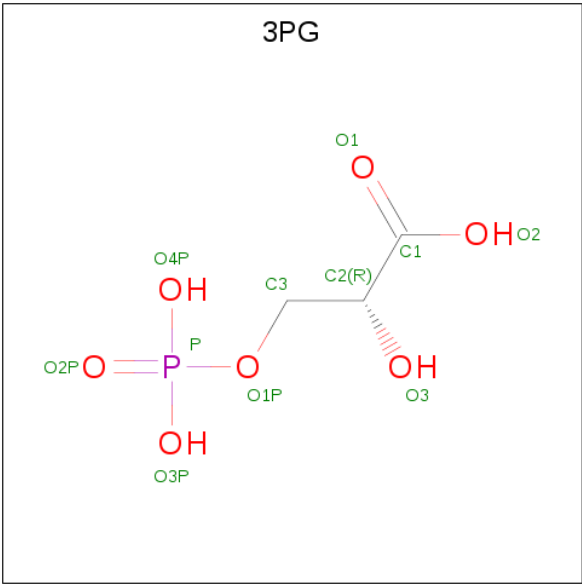
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is 3-PHOSPHOGLYCERIC ACID (three-letter code: 3PG) (formula: C₃H₇O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			11	3	7	1		
5	B	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 6 is water.

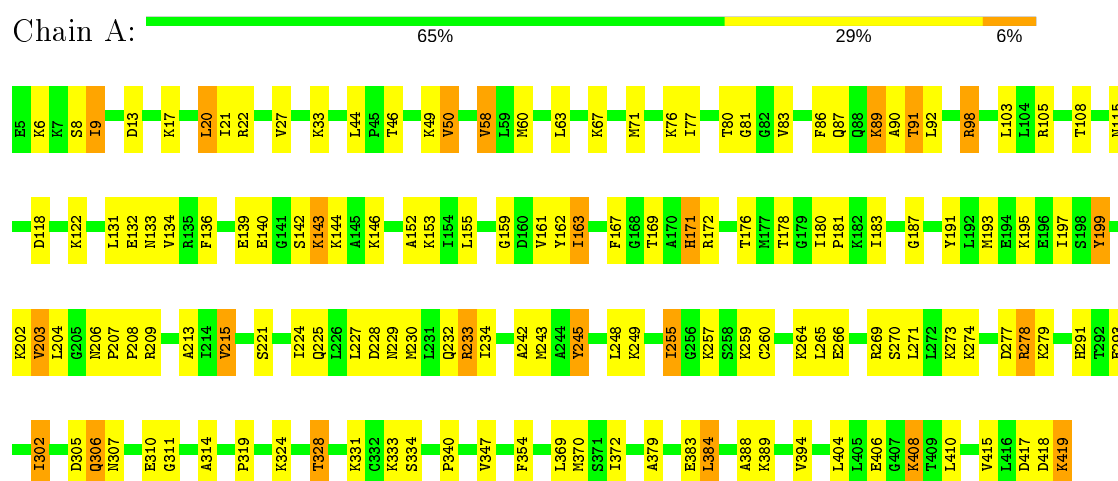
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	179	Total	O	0	0
			179	179		
6	B	164	Total	O	0	0
			164	164		
6	C	109	Total	O	0	0
			109	109		
6	D	147	Total	O	0	0
			147	147		

3 Residue-property plots

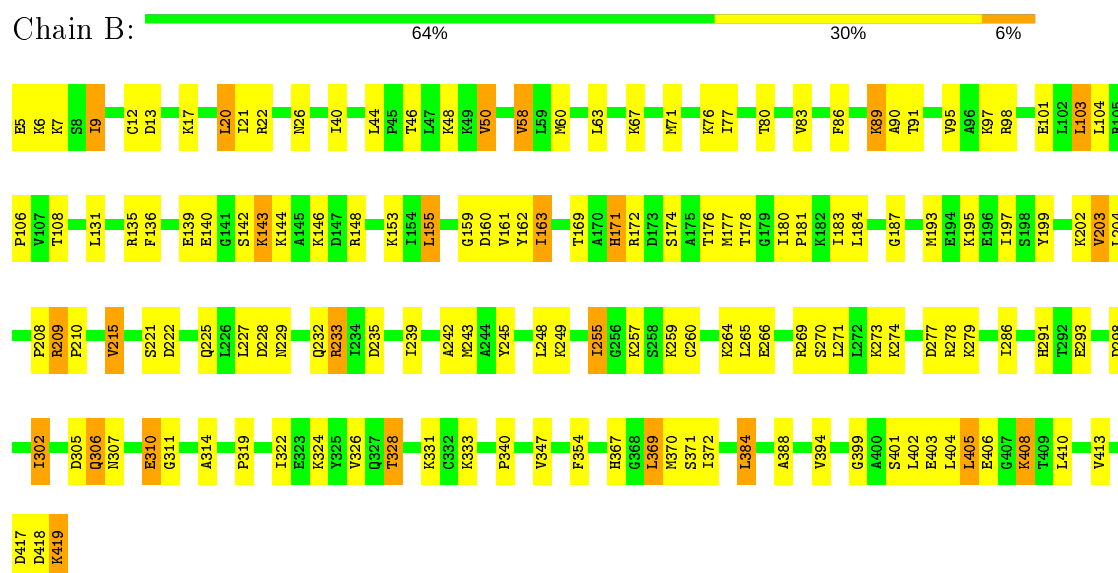
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: 3-PHOSPHOGLYCERATE KINASE

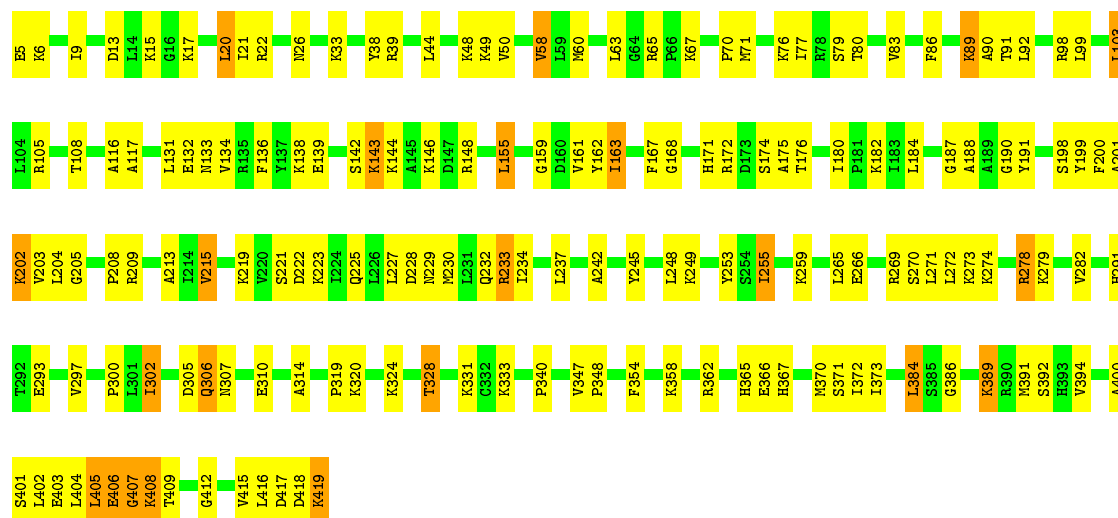


• Molecule 1: 3-PHOSPHOGLYCERATE KINASE



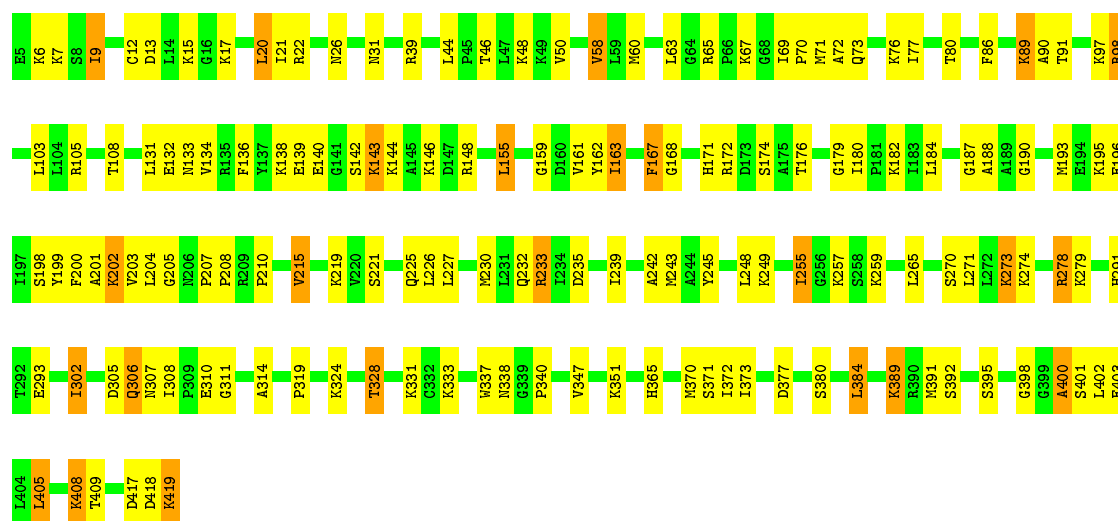
• Molecule 1: 3-PHOSPHOGLYCERATE KINASE





● Molecule 1: 3-PHOSPHOGLYCERATE KINASE

Chain D: 63% 31% 6%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.21Å 115.96Å 171.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	98.5 (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.221 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13271	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ADP, 3PG

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	0.57	0/3178	0.75	1/4273 (0.0%)
1	B	0.57	0/3178	0.73	0/4273
1	C	0.53	0/3178	0.72	2/4273 (0.0%)
1	D	0.55	0/3178	0.73	3/4273 (0.1%)
All	All	0.56	0/12712	0.73	6/17092 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	PHE	N-CA-C	-6.08	94.59	111.00
1	C	205	GLY	N-CA-C	-5.82	98.55	113.10
1	D	205	GLY	N-CA-C	-5.38	99.66	113.10
1	D	400	ALA	N-CA-C	-5.29	96.72	111.00
1	D	167	PHE	N-CA-C	-5.19	96.99	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	245	TYR	Sidechain

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	3127	0	3248	133	26
1	B	3127	0	3248	142	14
1	C	3127	0	3248	153	3
1	D	3127	0	3248	134	4
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	0	1	0
3	C	15	0	0	3	0
3	D	5	0	0	2	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	2	0
5	A	11	0	4	0	0
5	B	11	0	4	2	0
6	A	179	0	0	16	4
6	B	164	0	0	17	16
6	C	109	0	0	14	1
6	D	147	0	0	13	0
All	All	13271	0	13048	537	35

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 21.

The worst 5 of 537 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:6:LYS:HA	1:B:418:ASP:HA	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:THR:HG21	6:A:777:HOH:O	1.70	0.92
1:D:340:PRO:HD2	4:D:421:ADP:H5'2	1.48	0.92
1:A:6:LYS:HA	1:A:418:ASP:HA	1.55	0.89
1:D:203:VAL:HG12	1:D:204:LEU:HD12	1.61	0.83

The worst 5 of 35 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:ND2	6:B:477:HOH:O[2_465]	0.71	1.49
1:A:279:LYS:CG	6:B:503:HOH:O[3_555]	1.00	1.20
1:A:118:ASP:OD2	6:B:449:HOH:O[2_465]	1.25	0.95
1:A:209:ARG:NH2	1:B:279:LYS:CG[3_555]	1.28	0.92
1:A:279:LYS:CD	6:B:503:HOH:O[3_555]	1.33	0.87

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	413/415 (100%)	396 (96%)	17 (4%)	0	100	100
1	B	413/415 (100%)	391 (95%)	22 (5%)	0	100	100
1	C	413/415 (100%)	391 (95%)	17 (4%)	5 (1%)	13	24
1	D	413/415 (100%)	391 (95%)	21 (5%)	1 (0%)	47	68
All	All	1652/1660 (100%)	1569 (95%)	77 (5%)	6 (0%)	34	54

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
1	D	201	ALA

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Mol	Chain	Res	Type
1	C	201	ALA
1	C	406	GLU
1	C	175	ALA

5.3.2 Protein sidechains ⓘ

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	336/336 (100%)	303 (90%)	33 (10%)	8	15
1	B	336/336 (100%)	301 (90%)	35 (10%)	7	13
1	C	336/336 (100%)	306 (91%)	30 (9%)	9	19
1	D	336/336 (100%)	306 (91%)	30 (9%)	9	19
All	All	1344/1344 (100%)	1216 (90%)	128 (10%)	8	17

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	298	ASP
1	C	50	VAL
1	D	278	ARG
1	B	306	GLN
1	B	405	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	306	GLN
1	C	206	ASN
1	D	365	HIS
1	B	367	HIS
1	C	171	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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
3	PO4	A	701	-	4,4,4	0.87	0	6,6,6	0.56	0
3	PO4	C	702	-	4,4,4	1.39	0	6,6,6	0.43	0
4	ADP	D	421	2	24,29,29	1.11	2 (8%)	29,45,45	1.66	4 (13%)
3	PO4	C	624	2	4,4,4	1.40	0	6,6,6	0.59	0
3	PO4	A	704	-	4,4,4	0.83	0	6,6,6	0.84	0
3	PO4	C	703	-	4,4,4	1.03	0	6,6,6	0.76	0
3	PO4	D	625	-	4,4,4	1.76	2 (50%)	6,6,6	0.25	0
5	3PG	B	423	-	7,10,10	1.58	1 (14%)	10,14,14	4.93	5 (50%)
4	ADP	B	421	-	24,29,29	1.29	3 (12%)	29,45,45	1.52	3 (10%)
4	ADP	A	421	-	24,29,29	1.16	2 (8%)	29,45,45	1.62	3 (10%)
5	3PG	A	423	-	7,10,10	1.34	1 (14%)	10,14,14	4.58	3 (30%)
4	ADP	C	421	-	24,29,29	1.20	3 (12%)	29,45,45	1.83	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
4	ADP	D	421	2	-	1/12/32/32	0/3/3/3
5	3PG	B	423	-	-	6/6/10/10	-
4	ADP	B	421	-	-	1/12/32/32	0/3/3/3
4	ADP	A	421	-	-	0/12/32/32	0/3/3/3
5	3PG	A	423	-	-	6/6/10/10	-
4	ADP	C	421	-	-	1/12/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	423	3PG	P-O1P	3.49	1.71	1.60
4	C	421	ADP	O4'-C1'	3.20	1.45	1.41
5	A	423	3PG	P-O1P	2.78	1.69	1.60
4	B	421	ADP	C5-N7	-2.77	1.29	1.39
4	C	421	ADP	C5-N7	-2.51	1.30	1.39

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	423	3PG	O1P-C3-C2	12.87	145.09	107.94
5	A	423	3PG	O1P-C3-C2	12.26	143.32	107.94
5	A	423	3PG	P-O1P-C3	6.90	137.31	118.30
5	B	423	3PG	P-O1P-C3	6.75	136.89	118.30
4	C	421	ADP	N3-C2-N1	-6.22	118.95	128.68

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	423	3PG	O3-C2-C3-O1P
5	B	423	3PG	C2-C3-O1P-P
5	B	423	3PG	C3-O1P-P-O2P
5	B	423	3PG	C3-O1P-P-O3P
5	B	423	3PG	C3-O1P-P-O4P

There are no ring outliers.

9 monomers are involved in 13 short contacts:

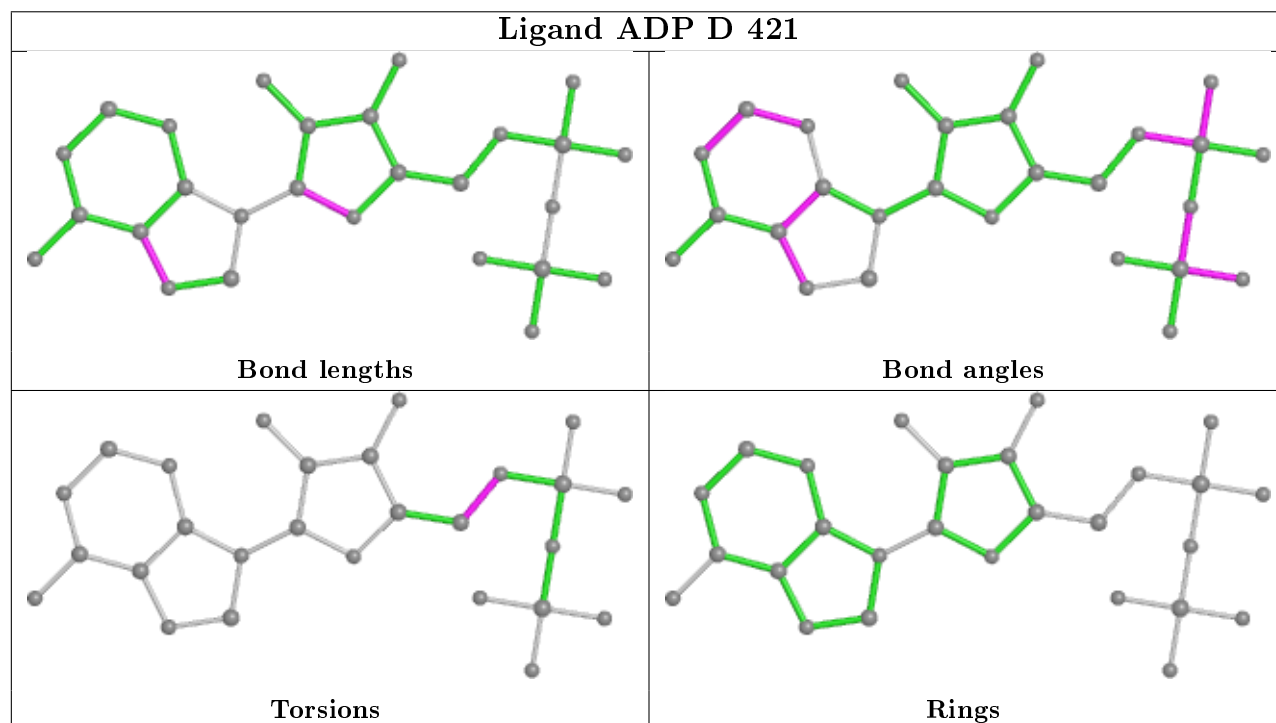
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	PO4	1	0

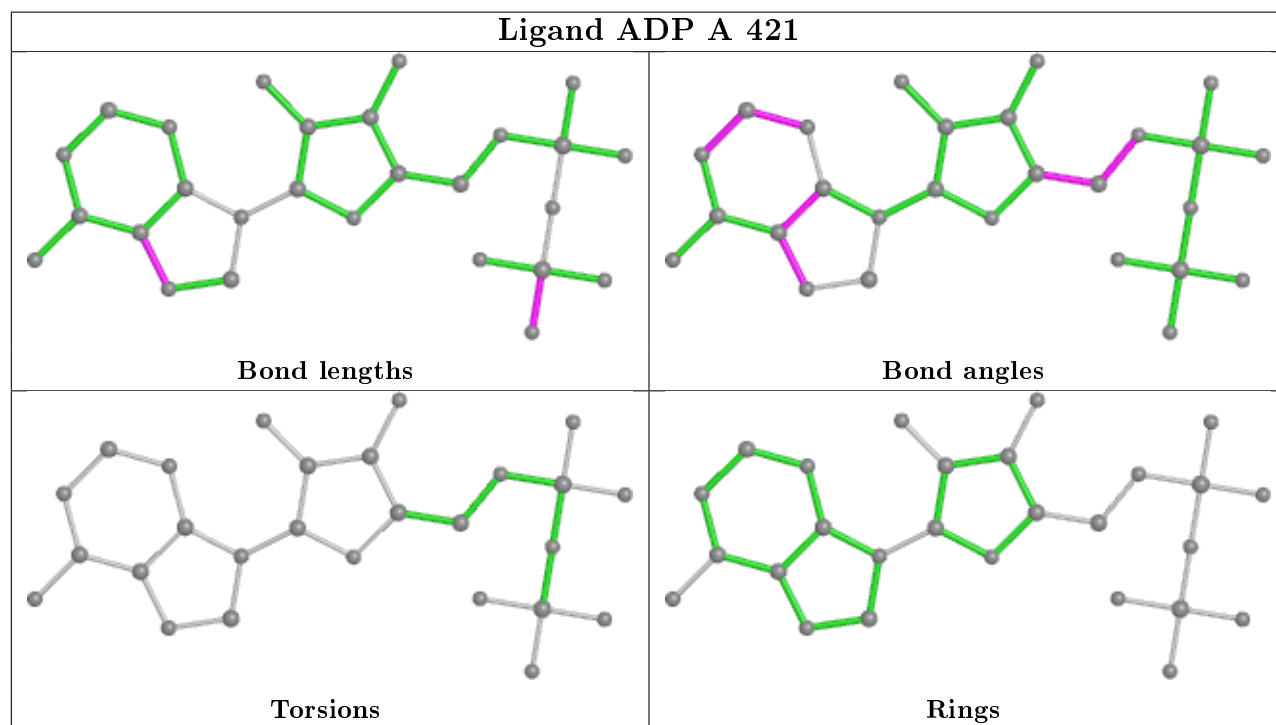
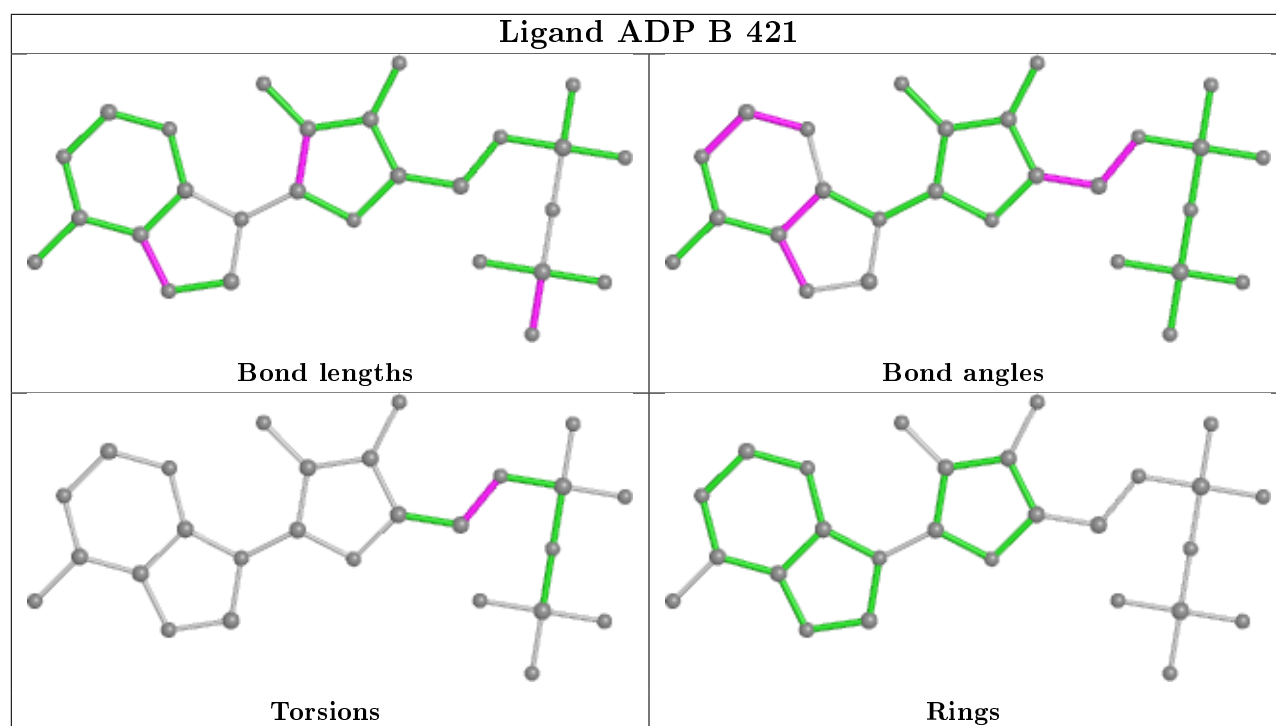
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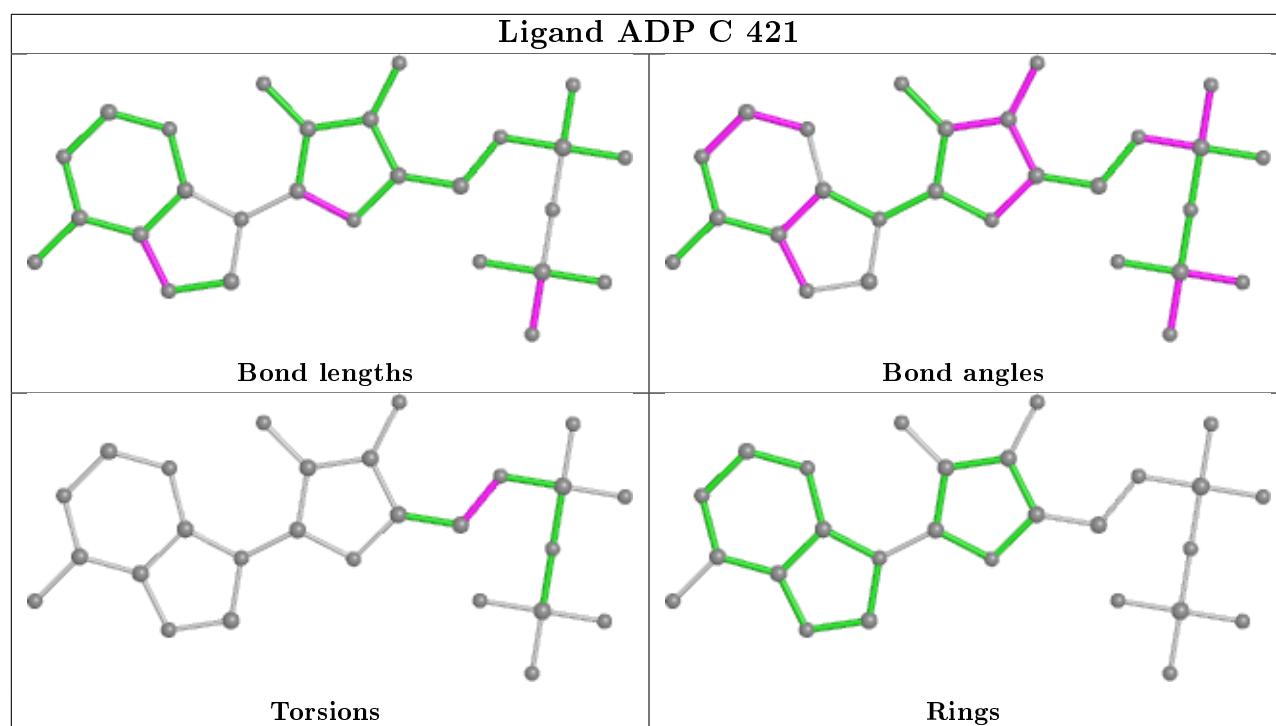
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	421	ADP	2	0
3	C	624	PO4	2	0
3	A	704	PO4	1	0
3	D	625	PO4	2	0
5	B	423	3PG	2	0
4	B	421	ADP	1	0
4	A	421	ADP	1	0
4	C	421	ADP	1	0

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 than 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.







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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.