



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 09:17 pm BST

PDB ID : 1GKI
Title : Plasmid coupling protein TrwB in complex with ADP and Mg²⁺.
Authors : Gomis-Ruth, F.X.; Moncalian, G.; De La cruz, F.; Coll, M.
Deposited on : 2001-08-14
Resolution : 3.00 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

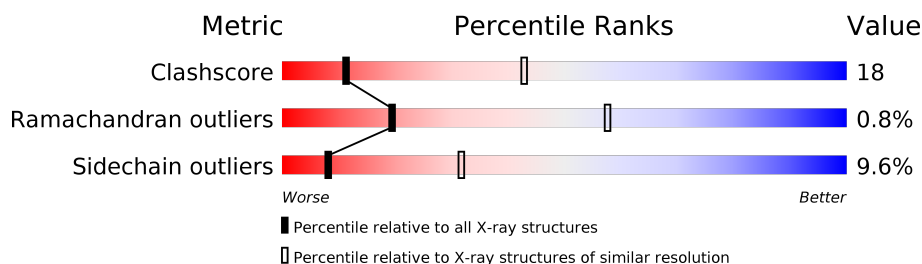
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	437	62% 29% 5%
1	B	437	61% 29% 5% 5%
1	D	437	61% 30% 5%
1	E	437	61% 29% 5% 5%
1	F	437	60% 30% 6%
1	G	437	59% 29% 5% 5%

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
4	EPE	E	1505	-	-	X	-

2 Entry composition [i](#)

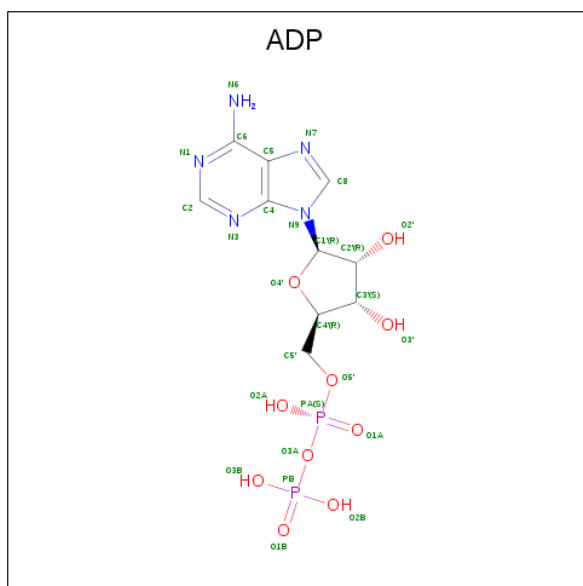
There are 5 unique types of molecules in this entry. The entry contains 20150 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CONJUGAL TRANSFER PROTEIN TRWB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3261	2063	582	606	10			
1	B	417	Total	C	N	O	S	0	0	0
			3274	2069	587	608	10			
1	D	416	Total	C	N	O	S	0	0	0
			3269	2067	586	606	10			
1	E	414	Total	C	N	O	S	0	0	0
			3254	2059	581	604	10			
1	F	412	Total	C	N	O	S	0	0	0
			3237	2048	578	601	10			
1	G	413	Total	C	N	O	S	0	0	0
			3241	2050	579	602	10			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

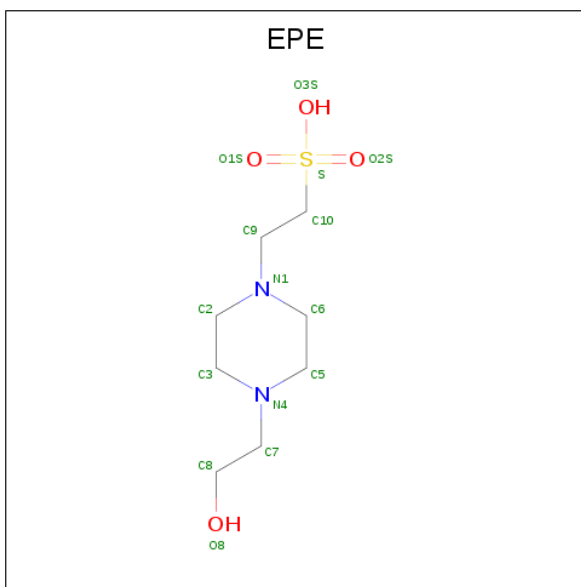


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

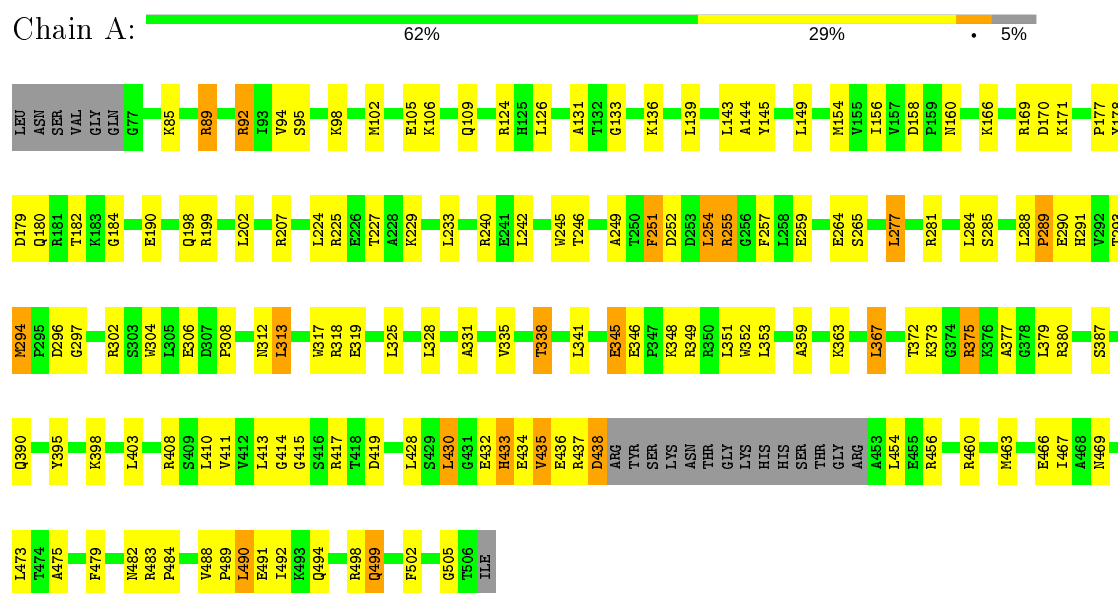
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	86	Total	O	0	0
			86	86		
5	D	85	Total	O	0	0
			85	85		
5	E	75	Total	O	0	0
			75	75		
5	F	51	Total	O	0	0
			51	51		
5	G	48	Total	O	0	0
			48	48		

3 Residue-property plots

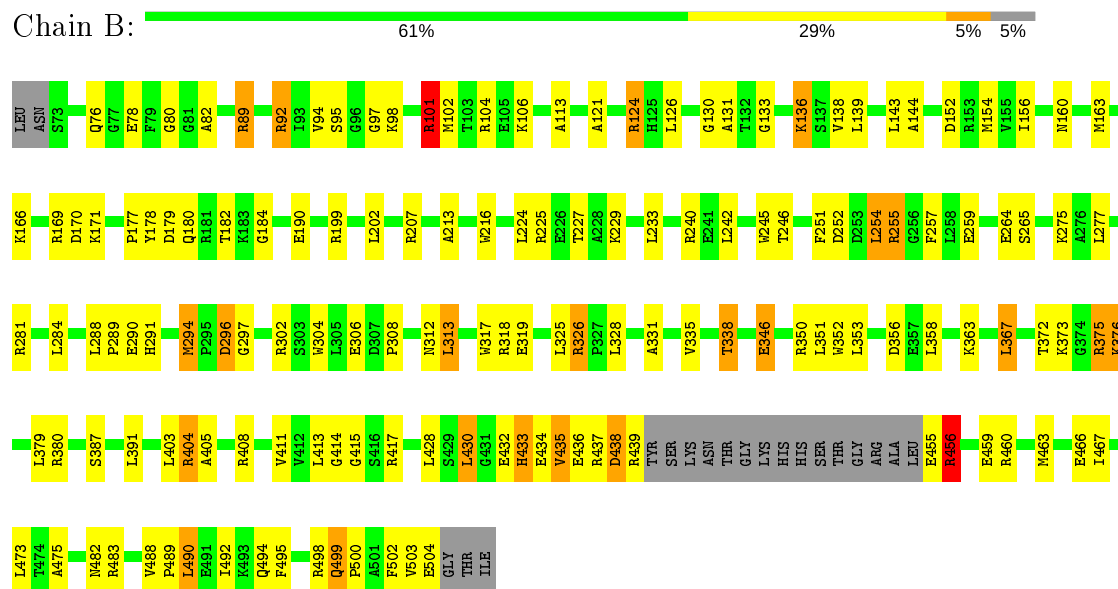
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

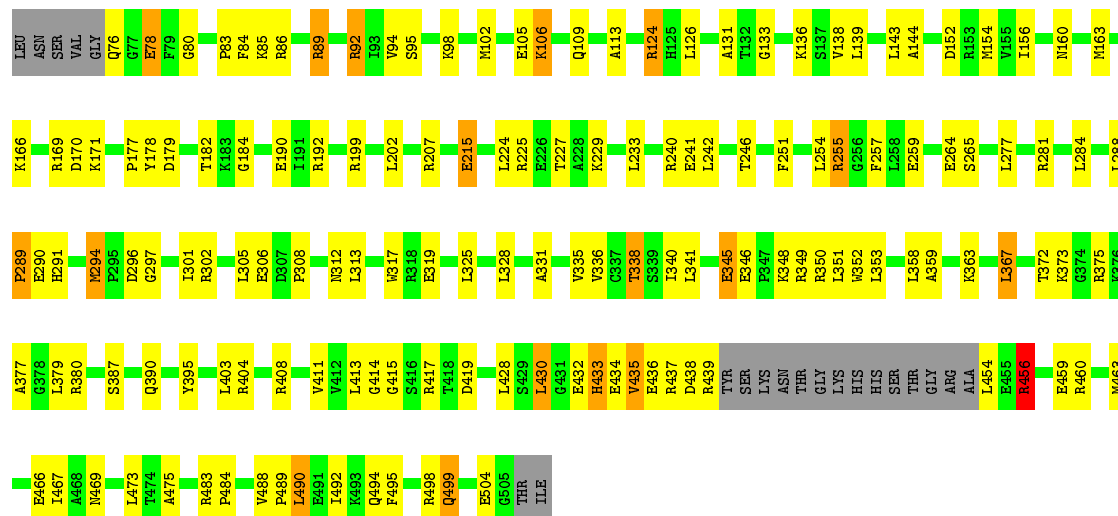


• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB



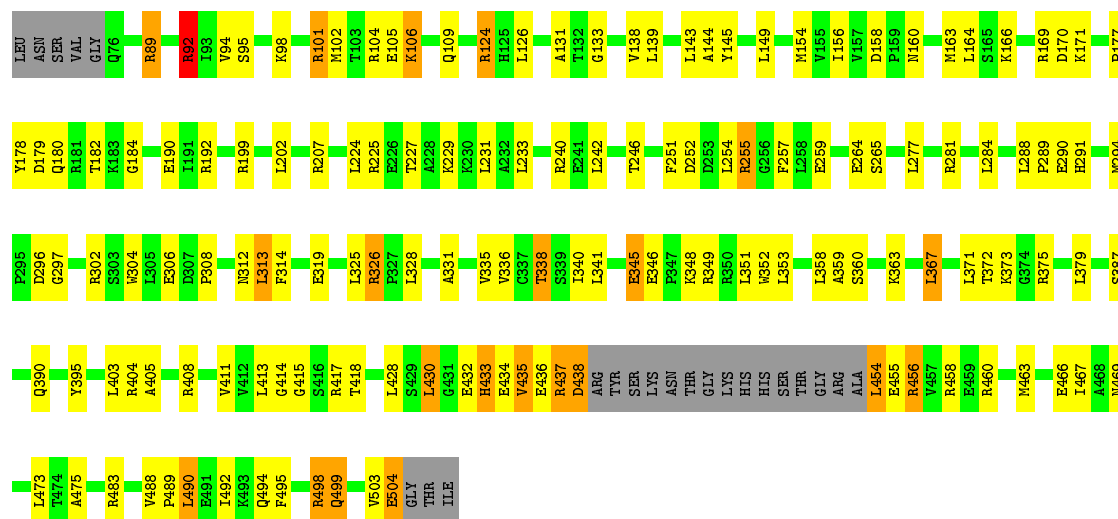
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain D: 



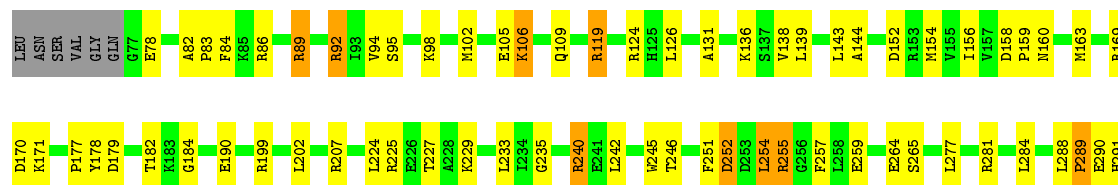
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

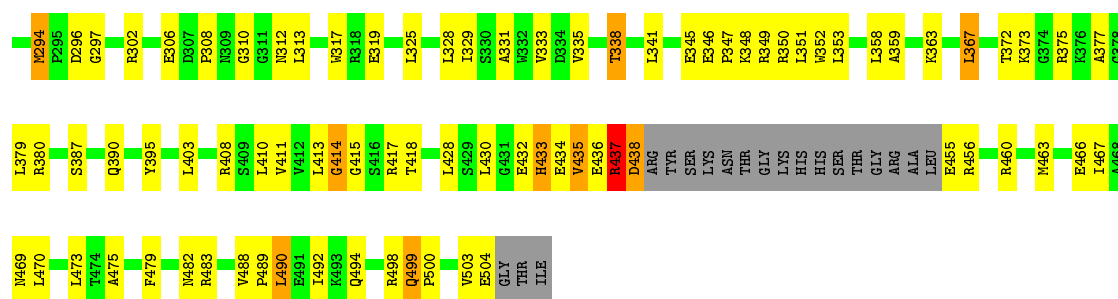
Chain E: 



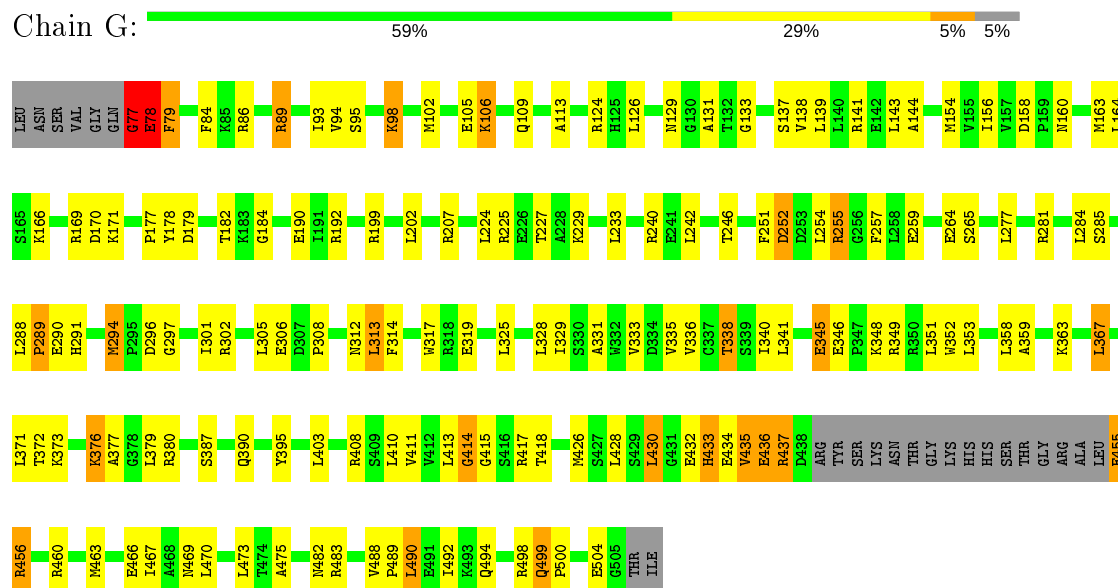
• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB

Chain F: 





• Molecule 1: CONJUGAL TRANSFER PROTEIN TRWB



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.10Å 151.10Å 251.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (50.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20150	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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: MG, EPE, ADP

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	0.44	2/3325 (0.1%)	0.67	2/4495 (0.0%)
1	B	0.50	4/3338 (0.1%)	0.87	17/4511 (0.4%)
1	D	0.48	2/3333 (0.1%)	0.75	5/4504 (0.1%)
1	E	0.64	10/3318 (0.3%)	0.99	21/4485 (0.5%)
1	F	0.60	3/3301 (0.1%)	0.84	10/4462 (0.2%)
1	G	0.74	8/3305 (0.2%)	0.99	20/4467 (0.4%)
All	All	0.58	29/19920 (0.1%)	0.86	75/26924 (0.3%)

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	F	0	1
1	G	1	3
All	All	1	4

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	77	GLY	N-CA	23.99	1.82	1.46
1	G	79	PHE	CD2-CE2	11.51	1.62	1.39
1	E	456	ARG	CZ-NH1	-11.34	1.18	1.33
1	G	456	ARG	CG-CD	-9.10	1.29	1.51
1	E	92	ARG	CD-NE	-8.34	1.32	1.46

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	437	ARG	NE-CZ-NH1	-20.41	110.09	120.30
1	G	78	GLU	N-CA-C	19.56	163.82	111.00
1	G	77	GLY	CA-C-N	-17.42	78.87	117.20
1	B	92	ARG	NE-CZ-NH1	-15.42	112.59	120.30
1	E	456	ARG	NE-CZ-NH2	14.90	127.75	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	78	GLU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	437	ARG	Sidechain
1	G	77	GLY	Mainchain,Peptide
1	G	78	GLU	Mainchain

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	3261	0	3290	111	0
1	B	3274	0	3302	124	1
1	D	3269	0	3299	125	1
1	E	3254	0	3283	129	1
1	F	3237	0	3264	121	1
1	G	3241	0	3266	128	0
2	A	27	0	12	3	0
2	B	27	0	12	3	0
2	D	27	0	12	3	0
2	E	27	0	12	2	0
2	F	27	0	12	3	0
2	G	27	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
4	E	30	0	33	13	0
5	A	72	0	0	2	0
5	B	86	0	0	3	0
5	D	85	0	0	5	0
5	E	75	0	0	2	0
5	F	51	0	0	1	0
5	G	48	0	0	1	0
All	All	20150	0	19809	702	2

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 18.

The worst 5 of 702 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:G:77:GLY:CA	1:G:77:GLY:N	1.82	1.41
1:E:101:ARG:HH12	4:E:1505:EPE:H101	1.05	1.14
1:E:438:ASP:HB3	1:E:454:LEU:CD1	1.88	1.03
1:E:438:ASP:HB3	1:E:454:LEU:CG	1.90	1.01
1:B:98:LYS:O	1:B:102:MET:HG3	1.60	1.01

All (2) 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:B:98:LYS:NZ	1:D:241:GLU:OE2[4_456]	2.13	0.07
1:E:92:ARG:NH1	1:F:235:GLY:O[5_565]	2.19	0.01

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	412/437 (94%)	388 (94%)	21 (5%)	3 (1%)	22	60
1	B	413/437 (94%)	394 (95%)	17 (4%)	2 (0%)	29	68
1	D	412/437 (94%)	390 (95%)	19 (5%)	3 (1%)	22	60
1	E	410/437 (94%)	387 (94%)	20 (5%)	3 (1%)	22	60
1	F	408/437 (93%)	389 (95%)	16 (4%)	3 (1%)	22	60
1	G	409/437 (94%)	385 (94%)	19 (5%)	5 (1%)	13	48
All	All	2464/2622 (94%)	2333 (95%)	112 (4%)	19 (1%)	19	57

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	78	GLU
1	E	499	GLN
1	G	345	GLU
1	G	499	GLN
1	A	499	GLN

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	346/364 (95%)	314 (91%)	32 (9%)	9	34
1	B	348/364 (96%)	315 (90%)	33 (10%)	8	32
1	D	347/364 (95%)	315 (91%)	32 (9%)	9	34
1	E	346/364 (95%)	313 (90%)	33 (10%)	8	32
1	F	344/364 (94%)	310 (90%)	34 (10%)	8	30
1	G	344/364 (94%)	309 (90%)	35 (10%)	7	28
All	All	2075/2184 (95%)	1876 (90%)	199 (10%)	8	32

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	430	LEU

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Mol	Chain	Res	Type
1	E	294	MET
1	G	313	LEU
1	D	435	VAL
1	E	143	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	494	GLN
1	E	160	ASN
1	G	433	HIS
1	D	497	ASN
1	D	499	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 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
2	ADP	F	701	-	24,29,29	1.47	5 (20%)	29,45,45	0.91	1 (3%)
2	ADP	D	701	3	24,29,29	1.35	3 (12%)	29,45,45	0.88	0
2	ADP	B	701	3	24,29,29	1.45	4 (16%)	29,45,45	0.93	1 (3%)
4	EPE	E	1506	-	15,15,15	3.26	10 (66%)	18,20,20	3.11	8 (44%)
2	ADP	A	701	3	24,29,29	1.31	3 (12%)	29,45,45	0.93	0
2	ADP	G	701	3	24,29,29	2.47	8 (33%)	29,45,45	1.72	6 (20%)
2	ADP	E	701	3	24,29,29	1.44	4 (16%)	29,45,45	0.90	0
4	EPE	E	1505	-	15,15,15	1.73	3 (20%)	18,20,20	1.66	6 (33%)

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	ADP	F	701	-	-	2/12/32/32	0/3/3/3
2	ADP	D	701	3	-	2/12/32/32	0/3/3/3
2	ADP	B	701	3	-	3/12/32/32	0/3/3/3
4	EPE	E	1506	-	-	3/9/19/19	0/1/1/1
2	ADP	A	701	3	-	3/12/32/32	0/3/3/3
2	ADP	G	701	3	-	2/12/32/32	0/3/3/3
2	ADP	E	701	3	-	2/12/32/32	0/3/3/3
4	EPE	E	1505	-	-	3/9/19/19	0/1/1/1

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	ADP	C2-N3	7.87	1.44	1.32
4	E	1506	EPE	C6-N1	-6.34	1.29	1.46
4	E	1506	EPE	C3-N4	5.39	1.61	1.46
4	E	1506	EPE	C7-N4	-4.08	1.38	1.47
4	E	1505	EPE	C7-N4	3.92	1.56	1.47

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1506	EPE	C7-N4-C5	-6.10	95.64	111.23
4	E	1506	EPE	C9-N1-C6	-5.15	98.05	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1506	EPE	C5-N4-C3	-4.75	98.13	108.83
4	E	1506	EPE	C9-N1-C2	4.53	122.81	111.23
4	E	1506	EPE	O8-C8-C7	-4.14	94.02	111.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1505	EPE	C10-C9-N1-C2
4	E	1506	EPE	C10-C9-N1-C6
2	E	701	ADP	PA-O3A-PB-O2B
4	E	1505	EPE	N4-C7-C8-O8
4	E	1506	EPE	N4-C7-C8-O8

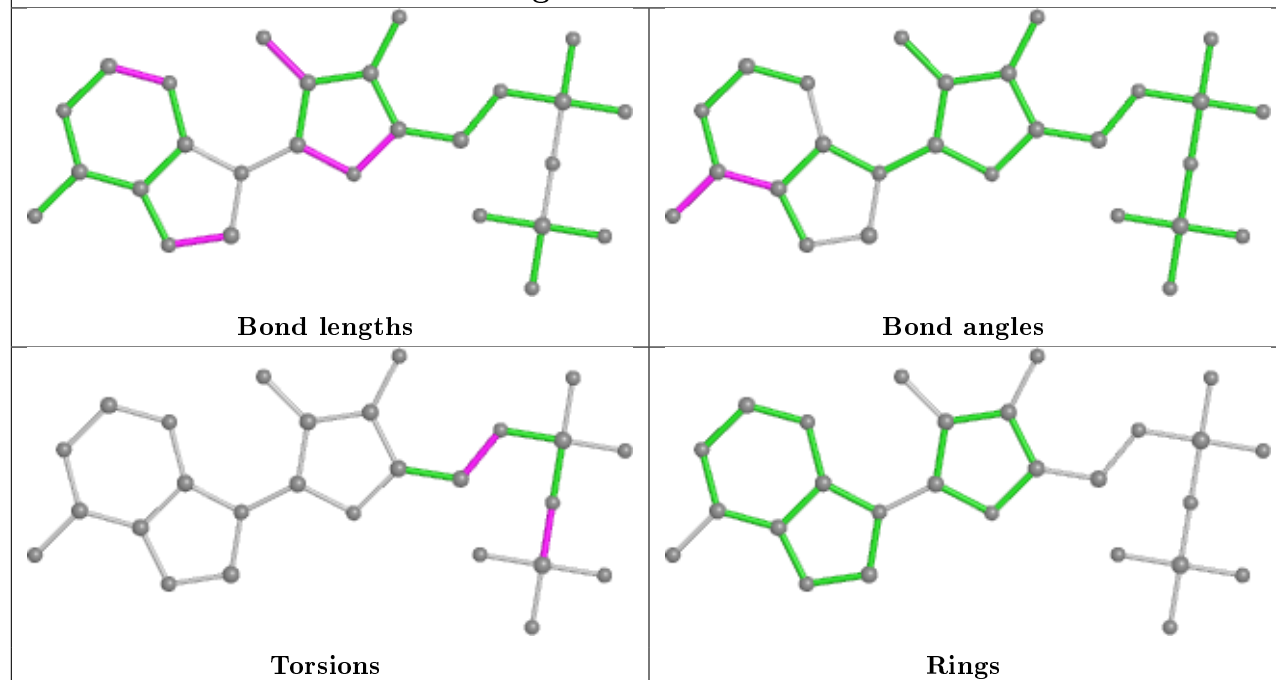
There are no ring outliers.

7 monomers are involved in 29 short contacts:

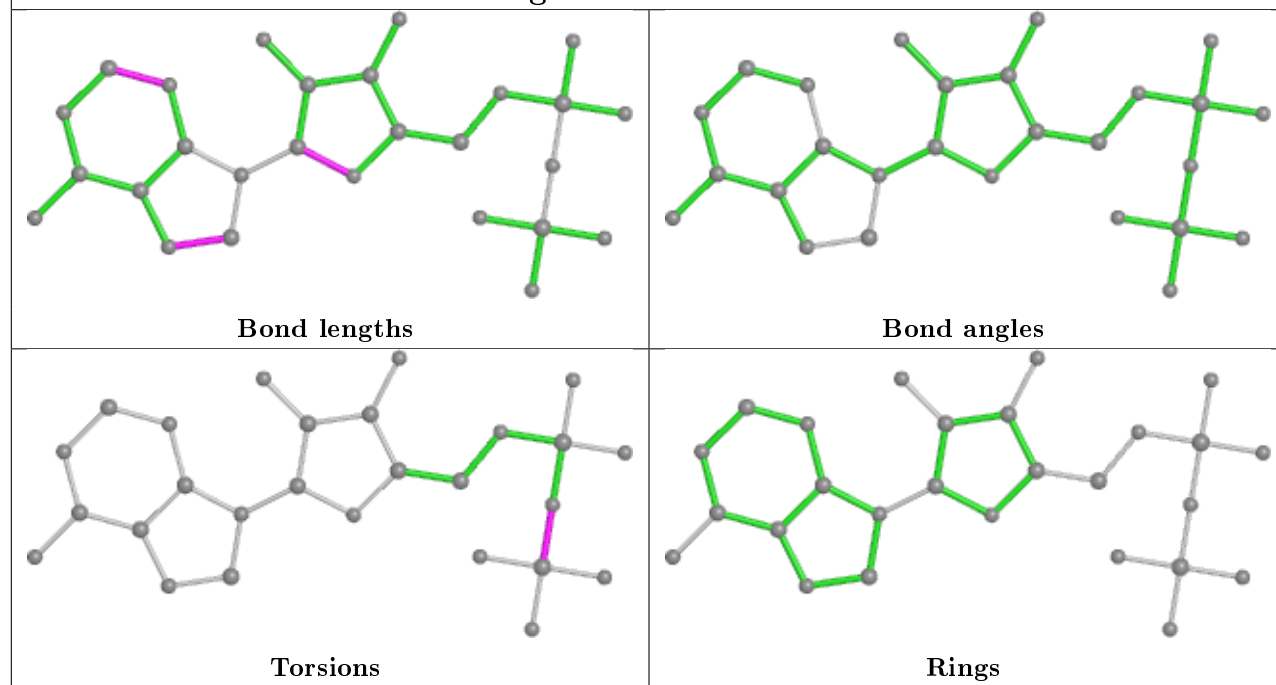
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	ADP	3	0
2	D	701	ADP	3	0
2	B	701	ADP	3	0
2	A	701	ADP	3	0
2	G	701	ADP	2	0
2	E	701	ADP	2	0
4	E	1505	EPE	13	0

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.

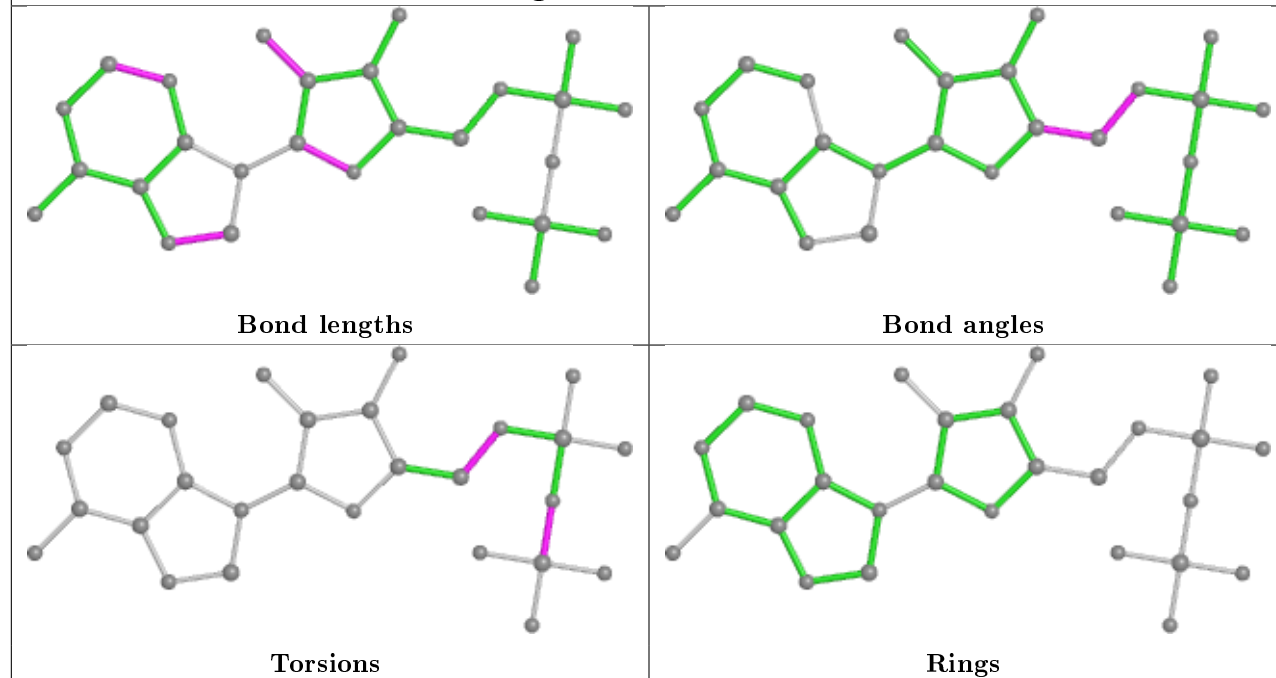
Ligand ADP F 701



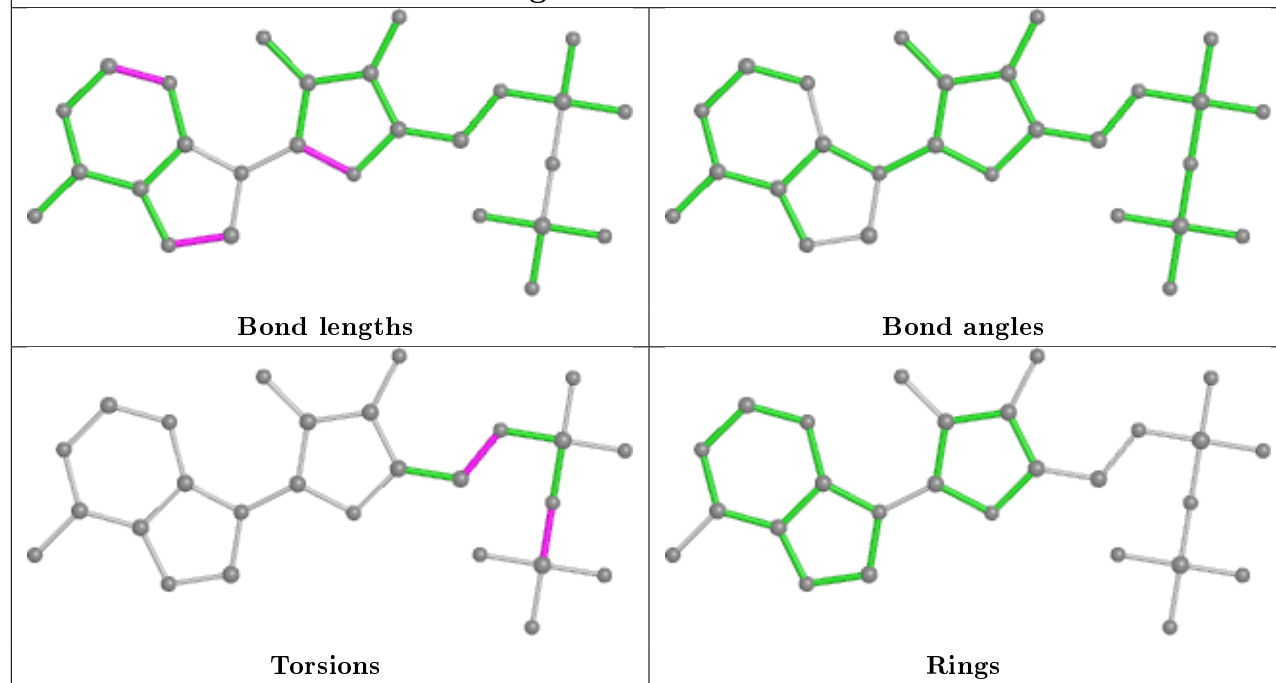
Ligand ADP D 701

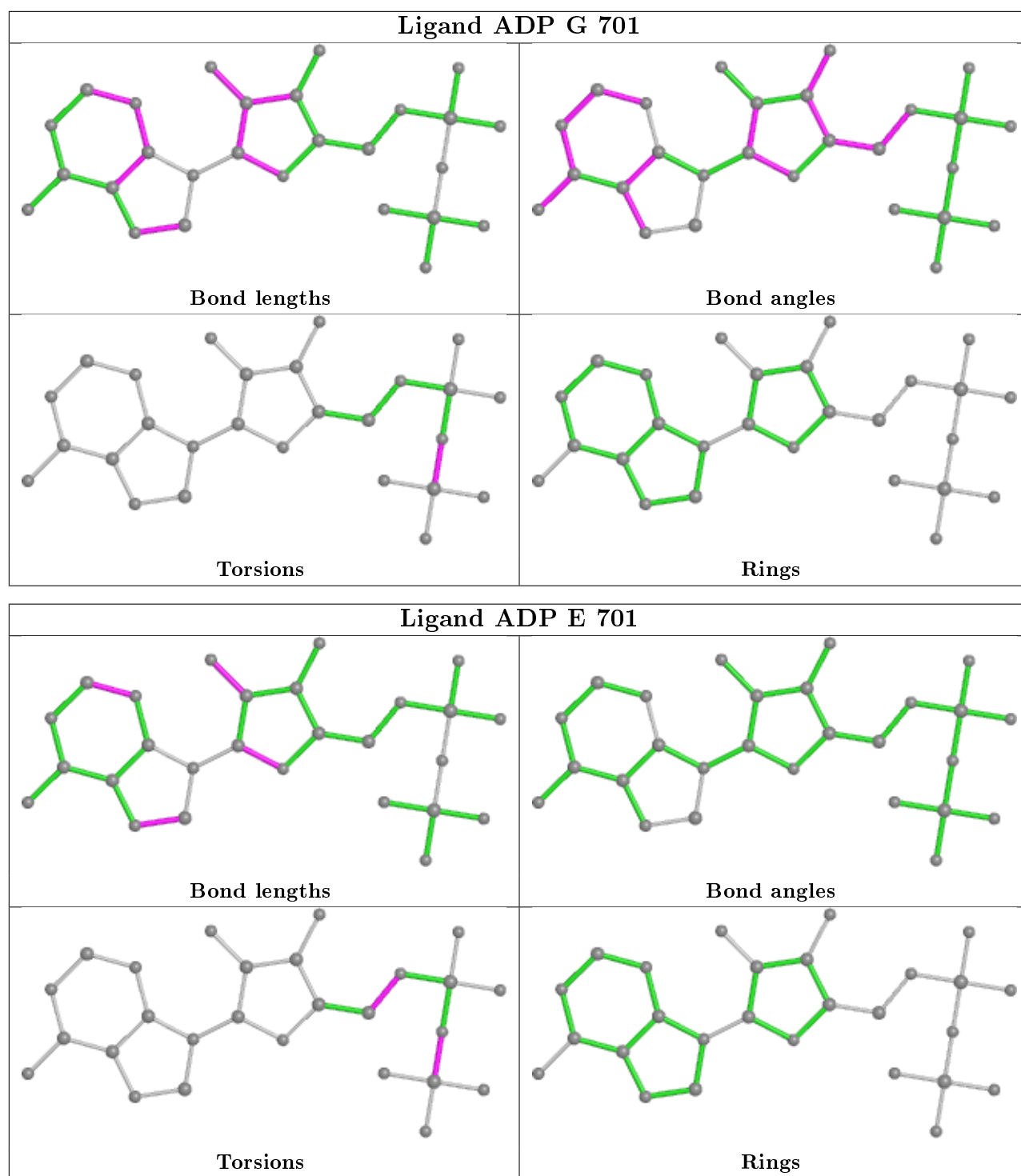


Ligand ADP B 701



Ligand ADP A 701





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.