wwPDB X-ray Structure Validation Summary Report (i)

Apr 29, 2024 – 02:20 pm BST

PDB ID	:	2CE7
Title	:	EDTA treated
Authors	:	Bieniossek, C.; Baumann, U.
Deposited on	:	2006-02-03
Resolution	:	2.44 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:

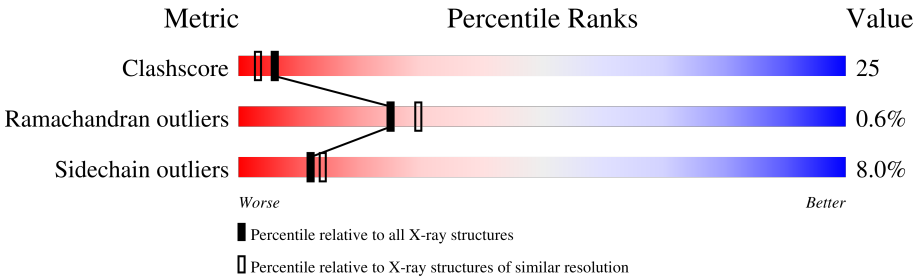
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.44 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	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	476	62% 20% · 14%
1	B	476	58% 25% · 14%
1	C	476	48% 36% · 12%
1	D	476	58% 25% · 13%
1	E	476	58% 23% · 15%
1	F	476	50% 32% 5% 13%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19564 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 CELL DIVISION PROTEIN FTSH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	1
			3160	1996	559	595	10			
1	B	411	Total	C	N	O	S	0	0	0
			3191	2017	560	604	10			
1	C	421	Total	C	N	O	S	0	0	0
			3280	2076	573	621	10			
1	D	413	Total	C	N	O	S	0	0	0
			3212	2032	562	608	10			
1	E	406	Total	C	N	O	S	0	0	1
			3144	1986	557	591	10			
1	F	412	Total	C	N	O	S	0	0	0
			3204	2024	564	606	10			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	ALA	LYS	engineered mutation	UNP Q9WZ49
B	410	LEU	LYS	engineered mutation	UNP Q9WZ49
B	415	ALA	LYS	engineered mutation	UNP Q9WZ49
C	415	ALA	LYS	engineered mutation	UNP Q9WZ49
D	410	LEU	LYS	engineered mutation	UNP Q9WZ49
D	415	ALA	LYS	engineered mutation	UNP Q9WZ49
E	410	LEU	LYS	engineered mutation	UNP Q9WZ49
E	415	ALA	LYS	engineered mutation	UNP Q9WZ49
F	415	ALA	LYS	engineered mutation	UNP Q9WZ49

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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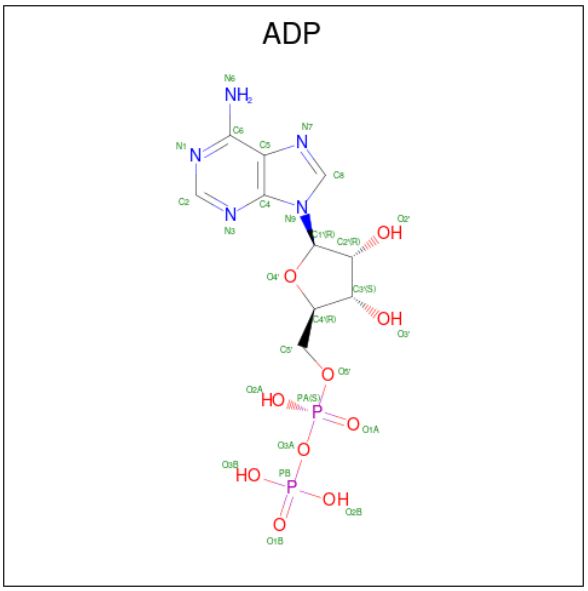
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- 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
3	A	1	Total C N O P 27 10 5 10 2	0	0
3	B	1	Total C N O P 27 10 5 10 2	0	0
3	C	1	Total C N O P 27 10 5 10 2	0	0
3	D	1	Total C N O P 27 10 5 10 2	0	0
3	E	1	Total C N O P 27 10 5 10 2	0	0
3	F	1	Total C N O P 27 10 5 10 2	0	0

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	46	Total O 46 46	0	0
5	B	33	Total O 33 33	0	0
5	C	26	Total O 26 26	0	0
5	D	33	Total O 33 33	0	0
5	E	38	Total O 38 38	0	0
5	F	23	Total O 23 23	0	0

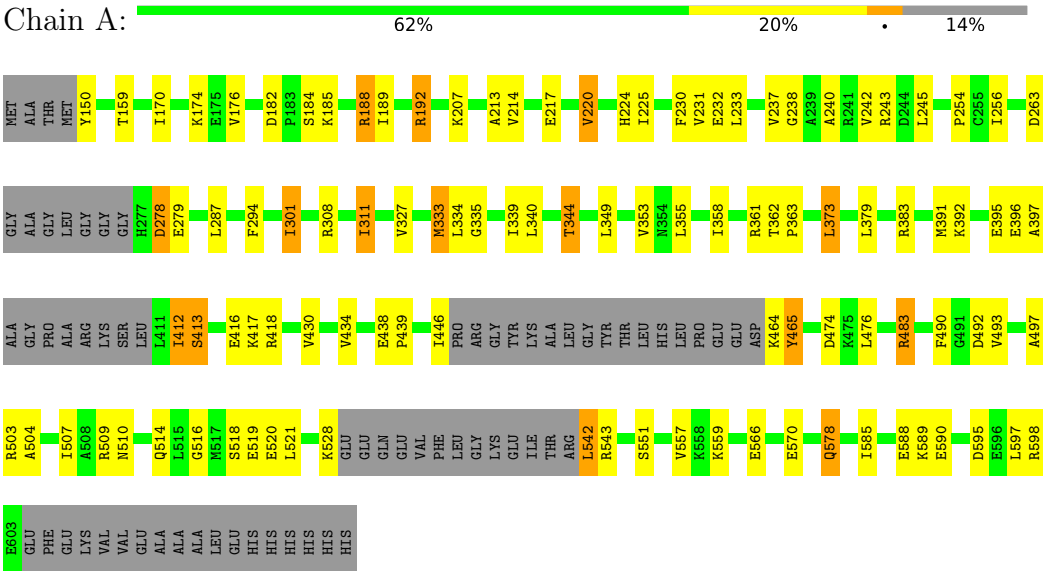
3 Residue-property plots (i)

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. 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.

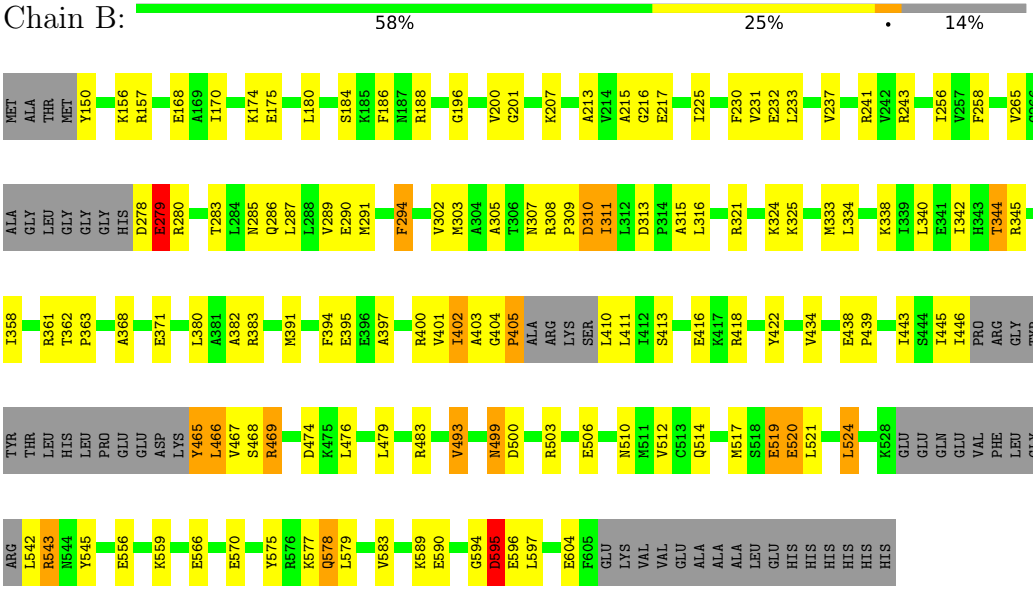
• Molecule 1: CELL DIVISION PROTEIN FTSH

Chain A:



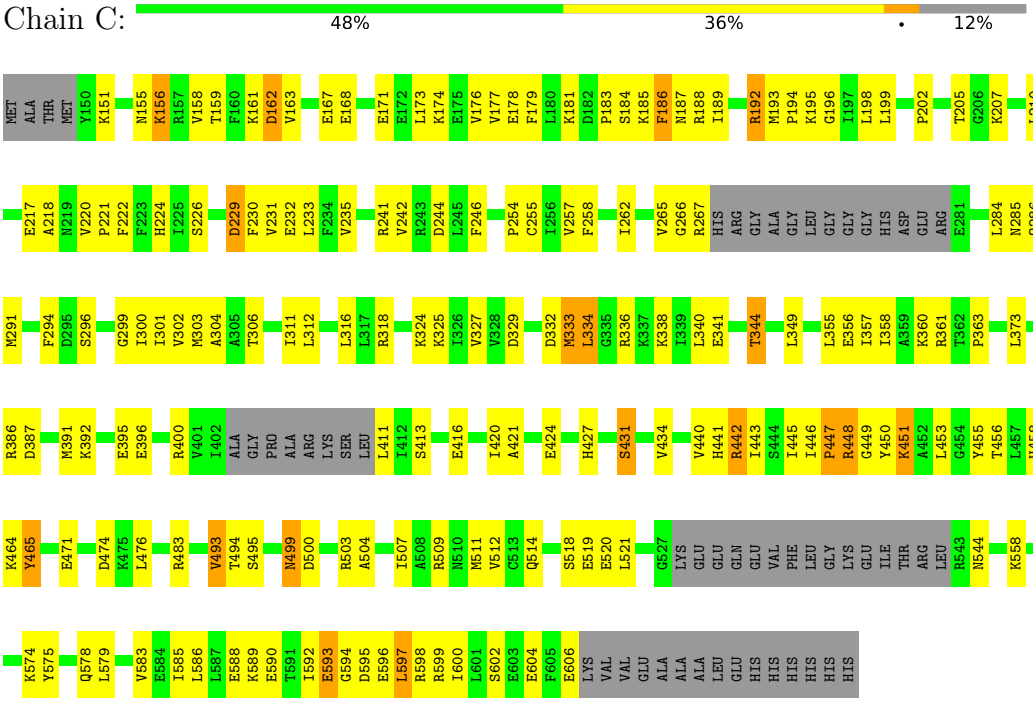
• Molecule 1: CELL DIVISION PROTEIN FTSH

Chain B:



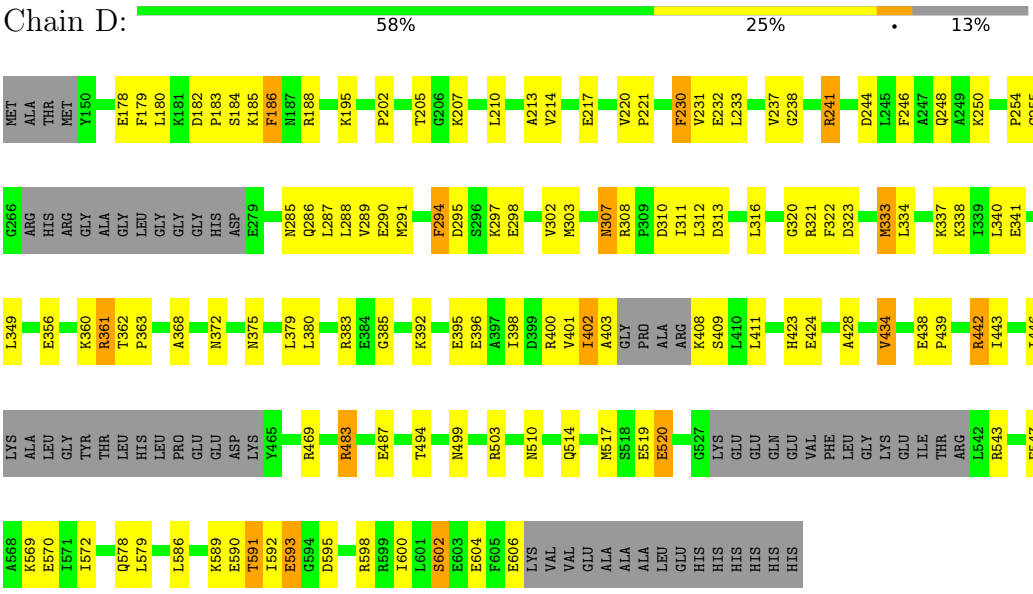
• Molecule 1: CELL DIVISION PROTEIN FTSH

Chain C:



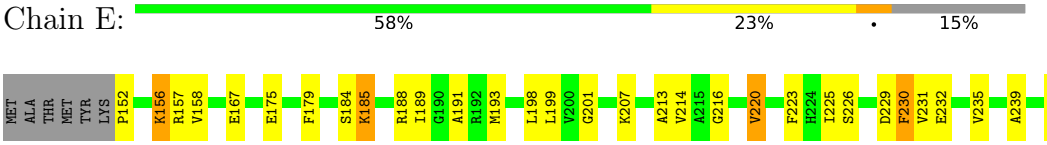
• Molecule 1: CELL DIVISION PROTEIN FTSH

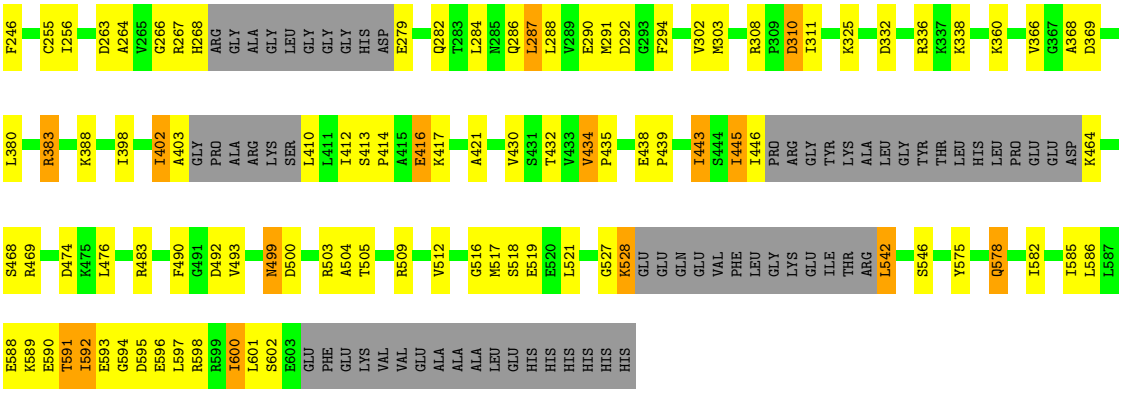
Chain D:



• Molecule 1: CELL DIVISION PROTEIN FTSH

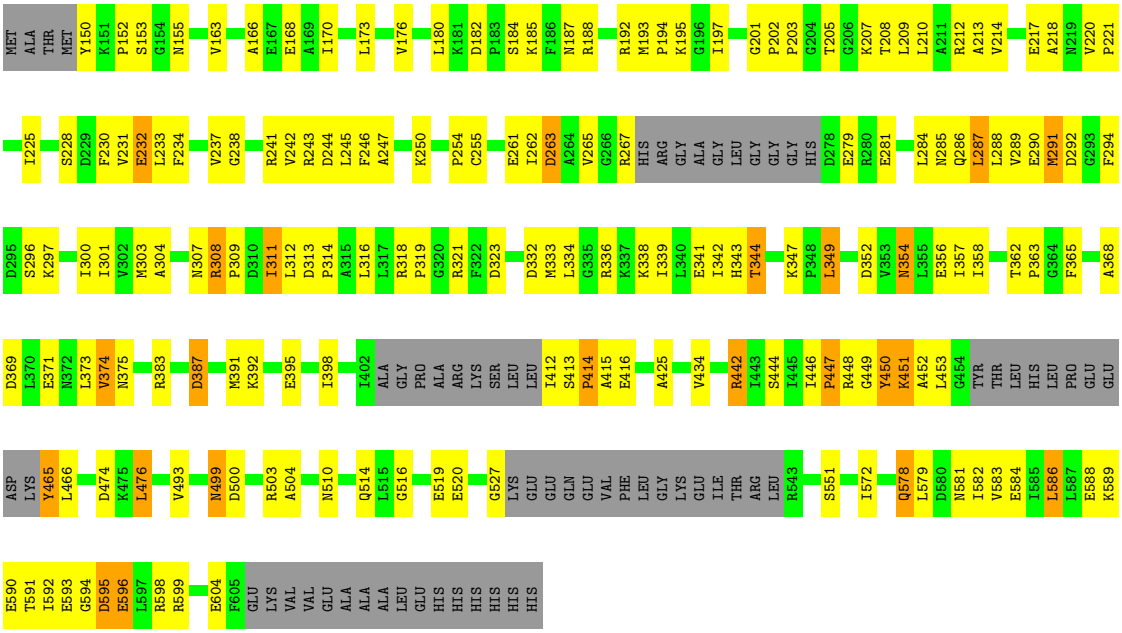
Chain E:





• Molecule 1: CELL DIVISION PROTEIN FTSH

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	165.09Å 165.09Å 235.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.44	Depositor
% Data completeness (in resolution range)	100.0 (25.00-2.44)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	19564	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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: ZN, ADP, 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	0.77	0/3202	0.60	1/4314 (0.0%)
1	B	0.74	2/3233 (0.1%)	0.55	1/4356 (0.0%)
1	C	0.61	0/3328	0.51	0/4488
1	D	0.69	0/3256	0.52	0/4388
1	E	0.71	1/3185 (0.0%)	0.54	0/4291
1	F	0.55	0/3248	0.47	0/4376
All	All	0.68	3/19452 (0.0%)	0.53	2/26213 (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	F	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	506	GLU	CG-CD	6.65	1.61	1.51
1	E	185	LYS	CD-CE	5.20	1.64	1.51
1	B	519	GLU	CG-CD	5.16	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	483	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	405	PRO	N-CA-CB	6.51	111.11	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	449	GLY	Peptide

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	3160	0	3240	111	0
1	B	3191	0	3261	125	0
1	C	3280	0	3346	225	0
1	D	3212	0	3283	125	0
1	E	3144	0	3231	157	0
1	F	3204	0	3270	237	0
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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	5	0
3	C	27	0	12	5	0
3	D	27	0	12	6	0
3	E	27	0	12	6	0
3	F	27	0	12	5	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	46	0	0	6	0
5	B	33	0	0	4	0
5	C	26	0	0	10	0
5	D	33	0	0	7	0
5	E	38	0	0	3	0
5	F	23	0	0	6	0
All	All	19564	0	19703	971	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 25.

The worst 5 of 971 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:C:340:LEU:O	1:C:344:THR:HG22	1.24	1.34
1:C:594:GLY:N	5:C:2024:HOH:O	1.60	1.29
1:A:446:ILE:HG22	5:A:2024:HOH:O	1.19	1.27
1:C:519:GLU:HA	5:C:2018:HOH:O	1.34	1.22
1:E:231:VAL:HG12	1:E:232:GLU:OE2	1.38	1.20

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	397/476 (83%)	383 (96%)	9 (2%)	5 (1%)	12	11
1	B	401/476 (84%)	385 (96%)	13 (3%)	3 (1%)	22	26
1	C	413/476 (87%)	392 (95%)	20 (5%)	1 (0%)	47	57
1	D	403/476 (85%)	387 (96%)	15 (4%)	1 (0%)	47	57
1	E	396/476 (83%)	380 (96%)	15 (4%)	1 (0%)	41	49
1	F	402/476 (84%)	381 (95%)	17 (4%)	4 (1%)	15	16
All	All	2412/2856 (84%)	2308 (96%)	89 (4%)	15 (1%)	25	29

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	TYR
1	A	602	SER
1	B	595	ASP

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Mol	Chain	Res	Type
1	F	414	PRO
1	A	601	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	337/390 (86%)	313 (93%)	24 (7%)	14 17
1	B	339/390 (87%)	314 (93%)	25 (7%)	13 16
1	C	349/390 (90%)	318 (91%)	31 (9%)	9 10
1	D	342/390 (88%)	317 (93%)	25 (7%)	14 17
1	E	335/390 (86%)	310 (92%)	25 (8%)	13 16
1	F	340/390 (87%)	307 (90%)	33 (10%)	8 8
All	All	2042/2340 (87%)	1879 (92%)	163 (8%)	12 14

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	416	GLU
1	F	383	ARG
1	E	499	ASN
1	F	234	PHE
1	F	499	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	354	ASN
1	F	375	ASN
1	F	514	GLN
1	D	372	ASN
1	D	307	ASN

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 18 ligands modelled in this entry, 12 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	$\#\|Z\| > 2$
3	ADP	B	1607	4	24,29,29	0.99	1 (4%)	29,45,45	1.42	4 (13%)
3	ADP	C	1608	4	24,29,29	1.05	3 (12%)	29,45,45	1.48	4 (13%)
3	ADP	F	1607	4	24,29,29	1.03	3 (12%)	29,45,45	1.51	4 (13%)
3	ADP	E	1604	4	24,29,29	0.91	1 (4%)	29,45,45	1.55	4 (13%)
3	ADP	A	1604	4	24,29,29	1.00	2 (8%)	29,45,45	1.34	2 (6%)
3	ADP	D	1608	4	24,29,29	1.19	2 (8%)	29,45,45	1.41	4 (13%)

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
3	ADP	B	1607	4	-	2/12/32/32	0/3/3/3
3	ADP	C	1608	4	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	F	1607	4	-	3/12/32/32	0/3/3/3
3	ADP	E	1604	4	-	3/12/32/32	0/3/3/3
3	ADP	A	1604	4	-	2/12/32/32	0/3/3/3
3	ADP	D	1608	4	-	3/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1608	ADP	C2'-C1'	-2.70	1.49	1.53
3	D	1608	ADP	C2-N3	2.52	1.36	1.32
3	F	1607	ADP	C2-N3	2.30	1.35	1.32
3	C	1608	ADP	C2-N3	2.26	1.35	1.32
3	A	1604	ADP	C5-C4	2.24	1.46	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1604	ADP	PA-O3A-PB	-4.70	116.68	132.83
3	A	1604	ADP	N3-C2-N1	-4.41	121.79	128.68
3	C	1608	ADP	N3-C2-N1	-4.12	122.24	128.68
3	E	1604	ADP	N3-C2-N1	-4.11	122.25	128.68
3	B	1607	ADP	N3-C2-N1	-4.06	122.34	128.68

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1604	ADP	C5'-O5'-PA-O3A
3	F	1607	ADP	C5'-O5'-PA-O1A
3	F	1607	ADP	C5'-O5'-PA-O2A
3	E	1604	ADP	O4'-C4'-C5'-O5'
3	E	1604	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1607	ADP	5	0
3	C	1608	ADP	5	0
3	F	1607	ADP	5	0

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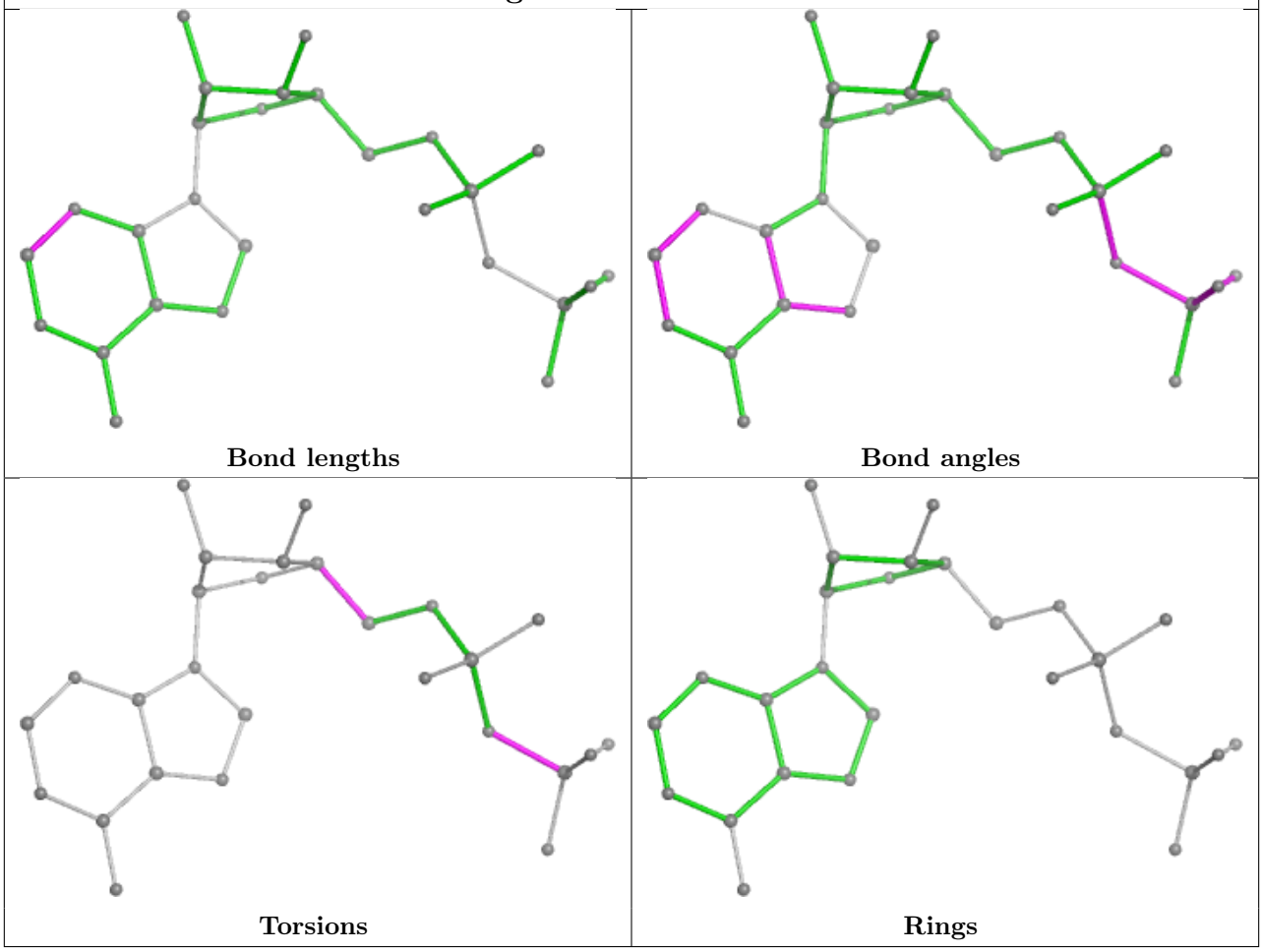
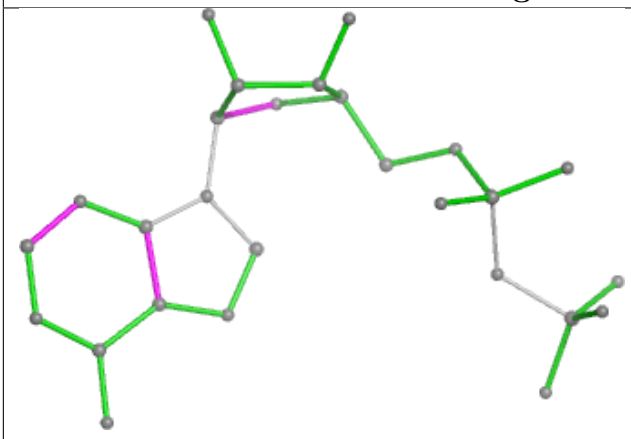
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1604	ADP	6	0
3	A	1604	ADP	3	0
3	D	1608	ADP	6	0

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.

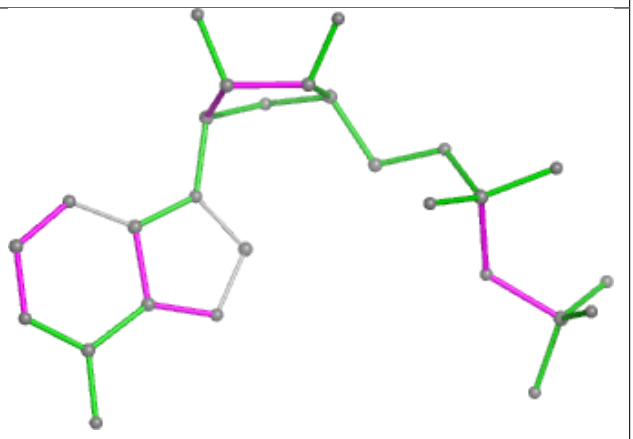
Ligand ADP B 1607



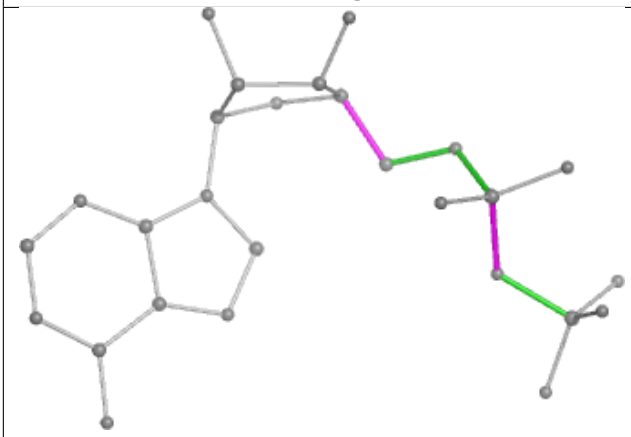
Ligand ADP C 1608



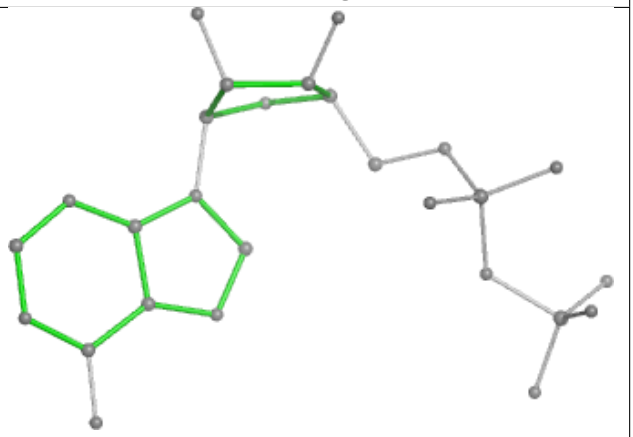
Bond lengths



Bond angles

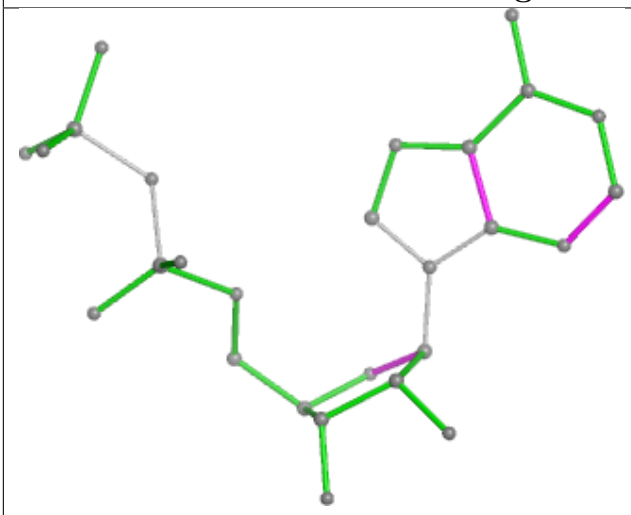


Torsions

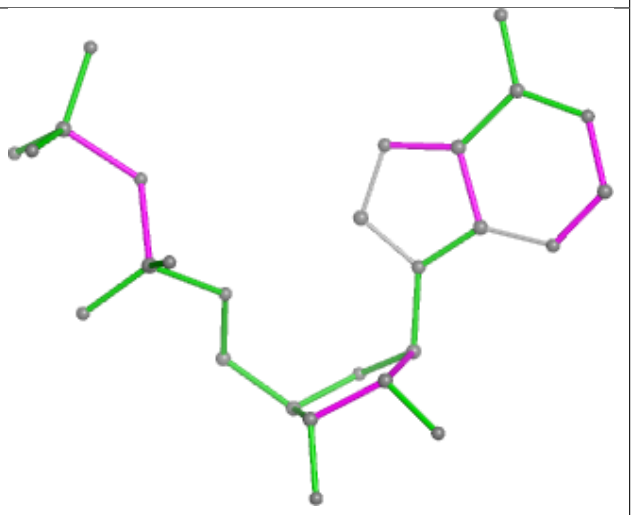


Rings

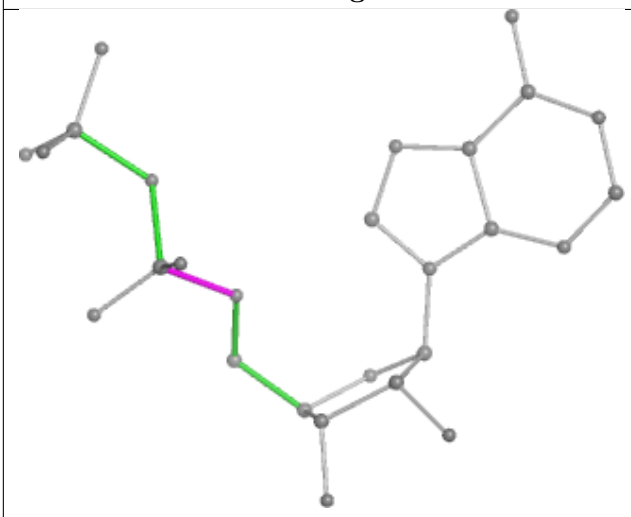
Ligand ADP F 1607



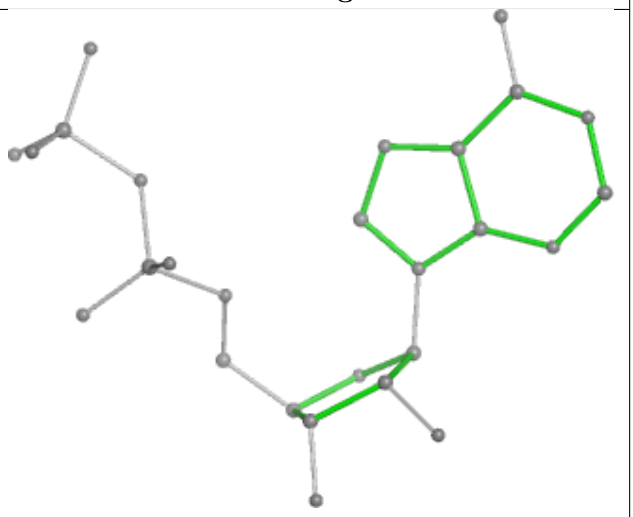
Bond lengths



Bond angles

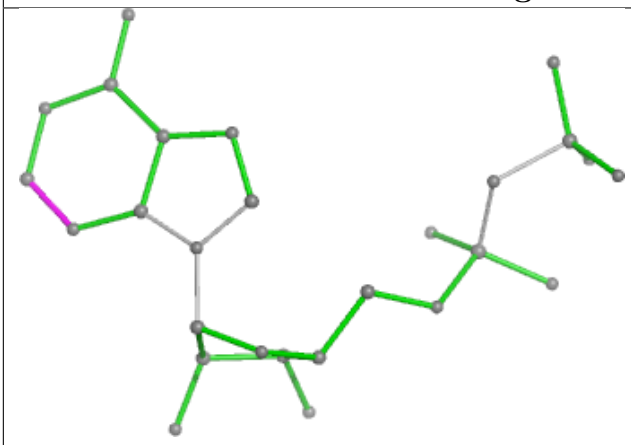


Torsions

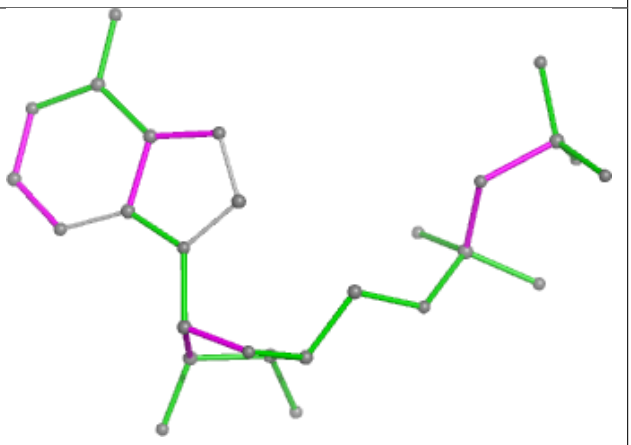


Rings

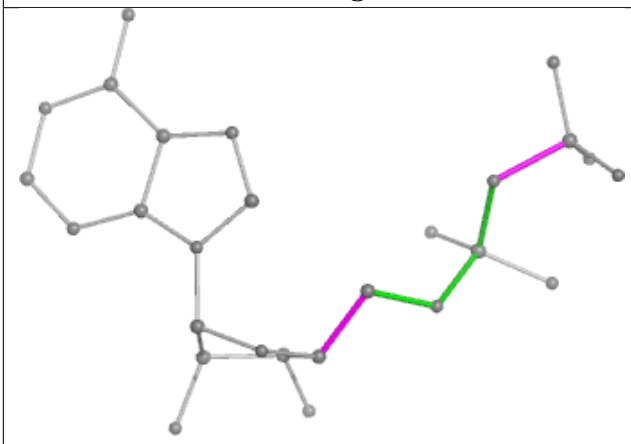
Ligand ADP E 1604



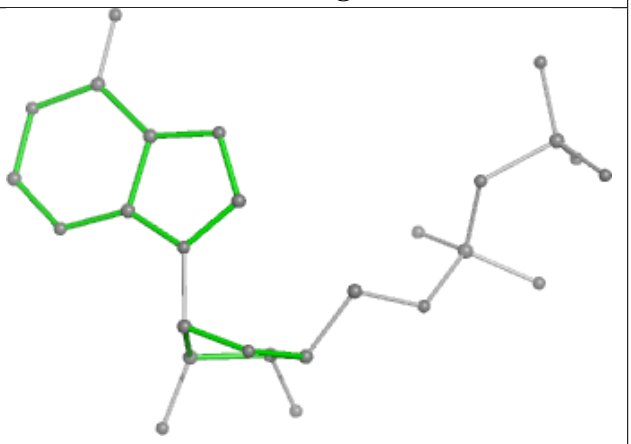
Bond lengths



Bond angles

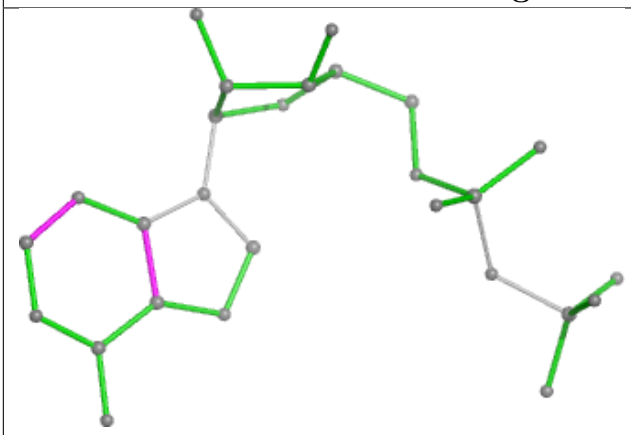


Torsions

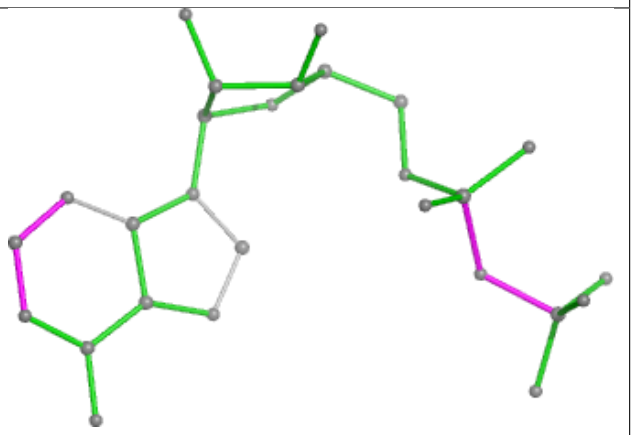


Rings

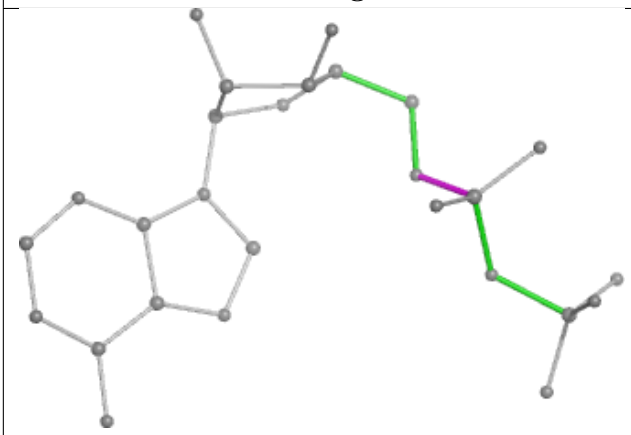
Ligand ADP A 1604



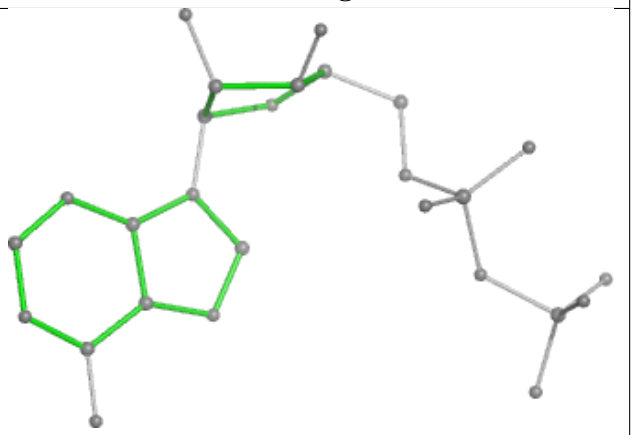
Bond lengths



Bond angles

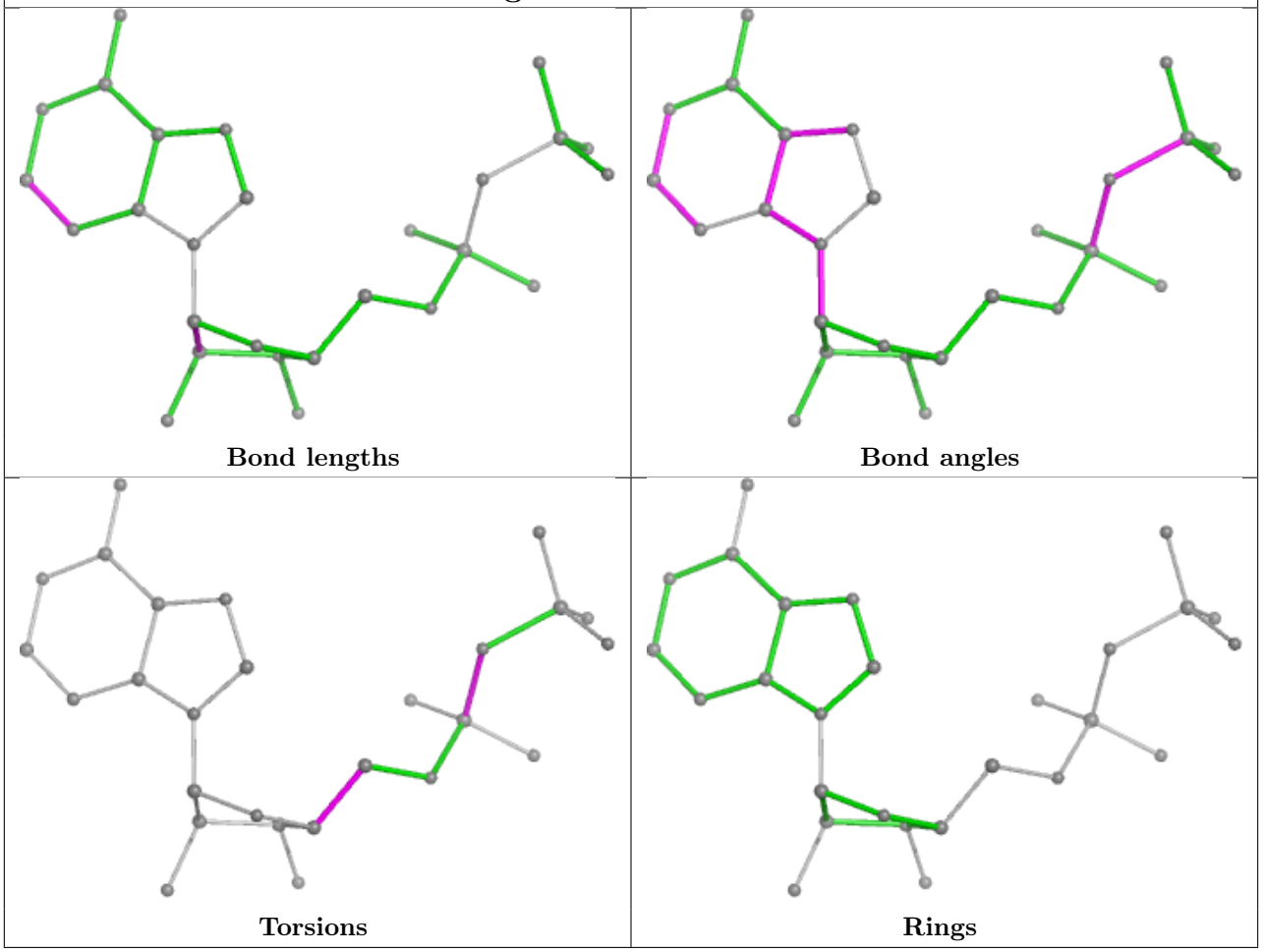


Torsions



Rings

Ligand ADP D 1608



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.