



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2024 – 01:58 AM EDT

PDB ID : 1T8S
Title : Crystal Structure of E.coli AMP Nucleosidase complexed with formicin 5'-monophosphate
Authors : Zhang, Y.; Cottet, S.E.; Ealick, S.E.
Deposited on : 2004-05-13
Resolution : 2.60 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 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

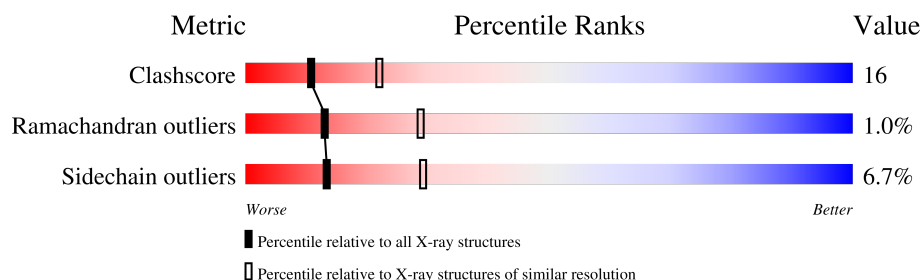
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	484	 65% 23% • 8%
1	B	484	 59% 29% • 8%
1	C	484	 64% 25% • 8%
1	D	484	 66% 23% • 8%
1	E	484	 63% 26% • 8%
1	F	484	 66% 23% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21455 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 AMP nucleosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	Se	0	0	0
			3505	2228	618	650	5	4			
1	B	444	Total	C	N	O	S	Se	0	0	0
			3514	2233	619	653	5	4			
1	C	443	Total	C	N	O	S	Se	0	0	0
			3505	2228	618	650	5	4			
1	D	443	Total	C	N	O	S	Se	0	0	0
			3505	2228	618	650	5	4			
1	E	443	Total	C	N	O	S	Se	0	0	0
			3505	2228	618	650	5	4			
1	F	443	Total	C	N	O	S	Se	0	0	0
			3505	2228	618	650	5	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MSE	MET	modified residue	UNP P15272
A	260	MSE	MET	modified residue	UNP P15272
A	302	MSE	MET	modified residue	UNP P15272
A	404	MSE	MET	modified residue	UNP P15272
B	138	MSE	MET	modified residue	UNP P15272
B	260	MSE	MET	modified residue	UNP P15272
B	302	MSE	MET	modified residue	UNP P15272
B	404	MSE	MET	modified residue	UNP P15272
C	138	MSE	MET	modified residue	UNP P15272
C	260	MSE	MET	modified residue	UNP P15272
C	302	MSE	MET	modified residue	UNP P15272
C	404	MSE	MET	modified residue	UNP P15272
D	138	MSE	MET	modified residue	UNP P15272
D	260	MSE	MET	modified residue	UNP P15272
D	302	MSE	MET	modified residue	UNP P15272
D	404	MSE	MET	modified residue	UNP P15272
E	138	MSE	MET	modified residue	UNP P15272

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Chain	Residue	Modelled	Actual	Comment	Reference
E	260	MSE	MET	modified residue	UNP P15272
E	302	MSE	MET	modified residue	UNP P15272
E	404	MSE	MET	modified residue	UNP P15272
F	138	MSE	MET	modified residue	UNP P15272
F	260	MSE	MET	modified residue	UNP P15272
F	302	MSE	MET	modified residue	UNP P15272
F	404	MSE	MET	modified residue	UNP P15272

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- The chemical structure of 5'-phosphoryl-UMP (FMP) is shown with the following atom labels:
- Nucleobase:** A pyrimidine ring with atoms N1, N3, N6 (NH₂), C2, C4, C5, and C6.
 - Sugar:** A ribose ring with atoms C1'(S), C2'(R), C3'(S), C4'(R), and C5'.
 - Phosphate:** A phosphate group attached to C5' via an oxygen atom (O5'). The phosphate group includes a phosphorus atom (P) and non-hydroxyl oxygens O1P and O3P.
 - Hydroxyl Groups:** Two hydroxyl groups are attached to the sugar ring at C2' (O2') and C3' (O3').
- The stereochemistry at the sugar ring is indicated by (S) and (R) labels at C1', C2', C3', and C4'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	D	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	E	1	Total 23	C 10	N 5	O 7	P 1	0	0
2	F	1	Total 23	C 10	N 5	O 7	P 1	0	0

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- WORLD WIDE
PDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total 44	O 44	0	0
3	B	43	Total 43	O 43	0	0
3	C	42	Total 42	O 42	0	0
3	D	71	Total 71	O 71	0	0
3	E	46	Total 46	O 46	0	0
3	F	32	Total 32	O 32	0	0

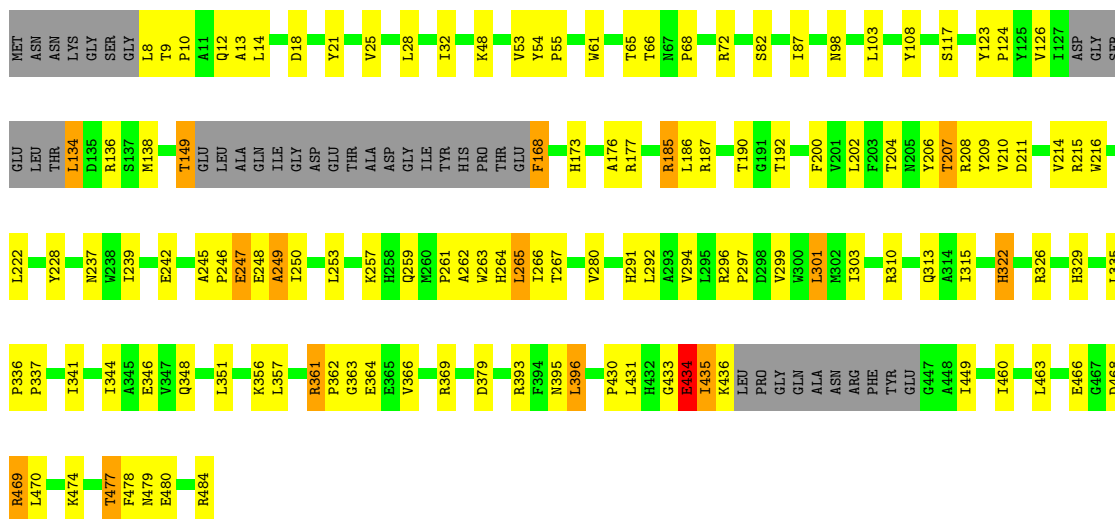
3 Residue-property plots

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.

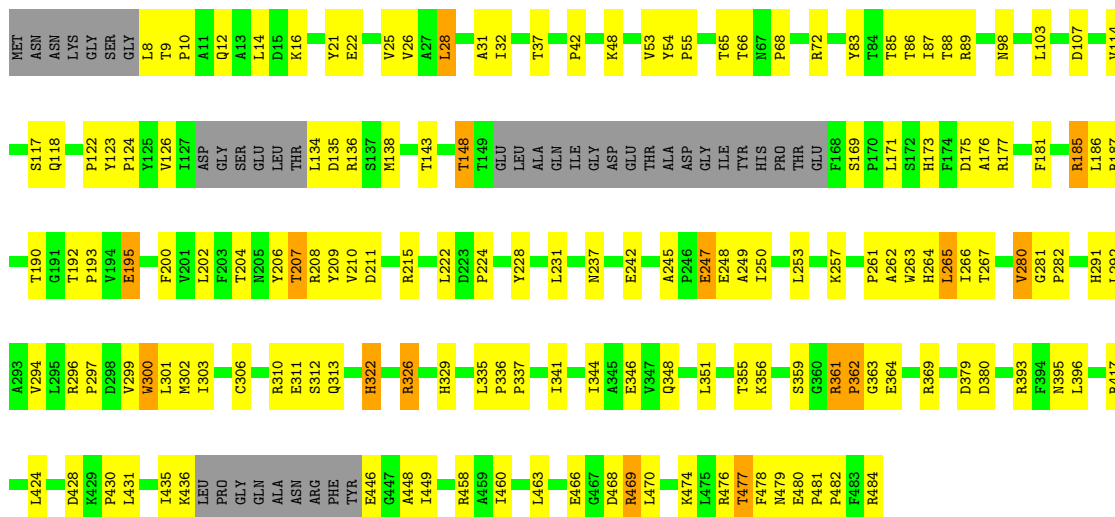
• Molecule 1: AMP nucleosidase

Chain A: 



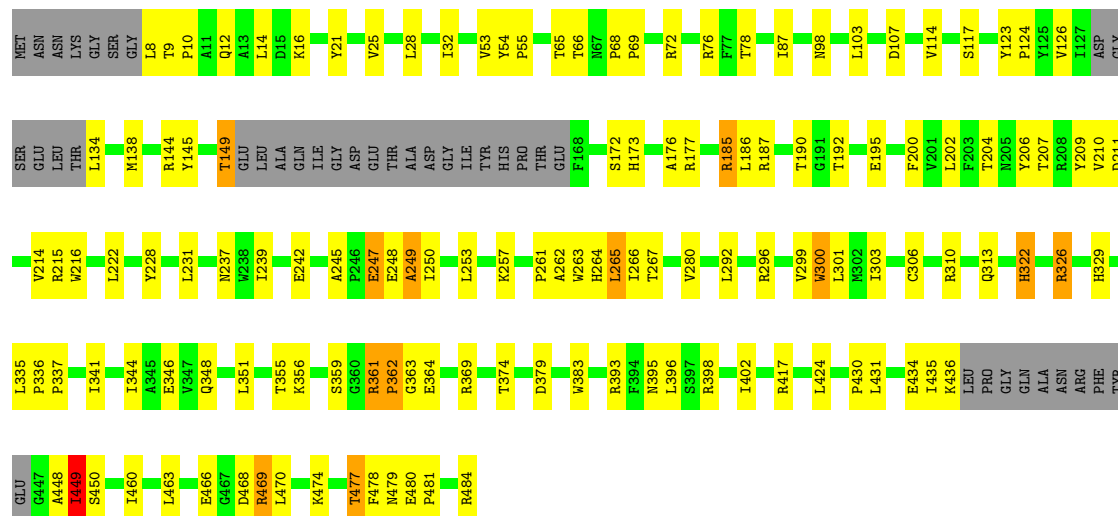
• Molecule 1: AMP nucleosidase

Chain B: 



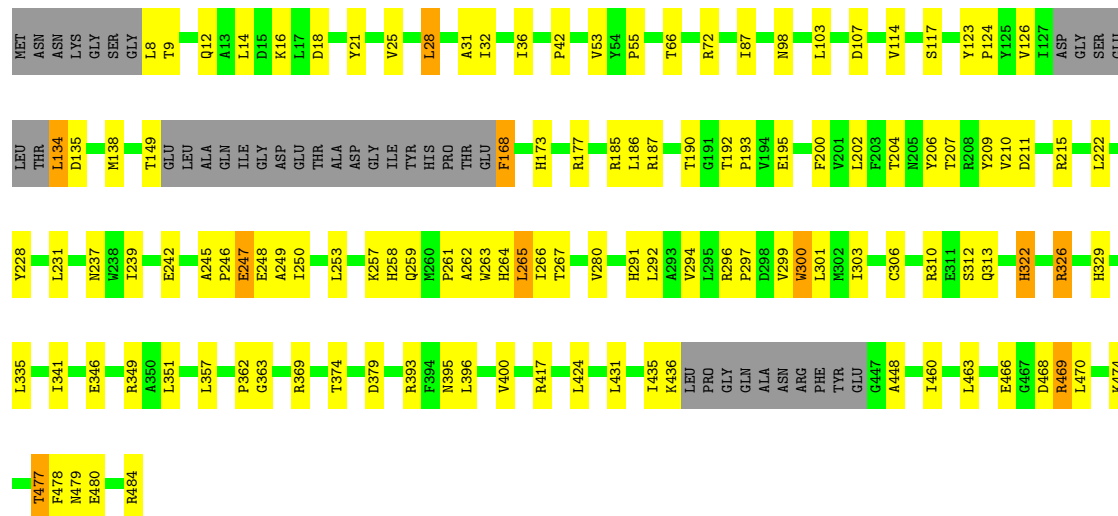
- Molecule 1: AMP nucleosidase

Chain C: 



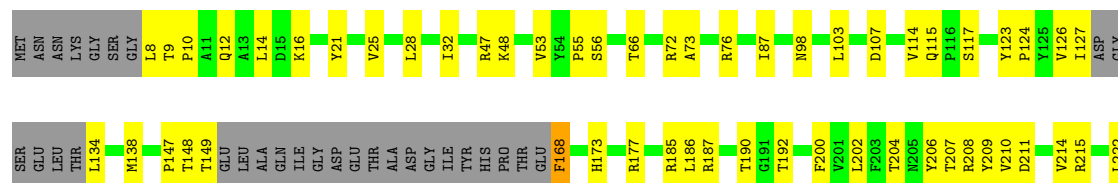
- Molecule 1: AMP nucleosidase

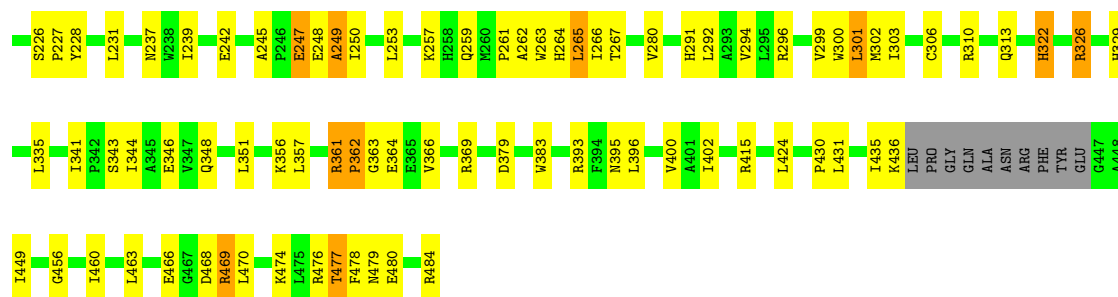
Chain D: 



- Molecule 1: AMP nucleosidase

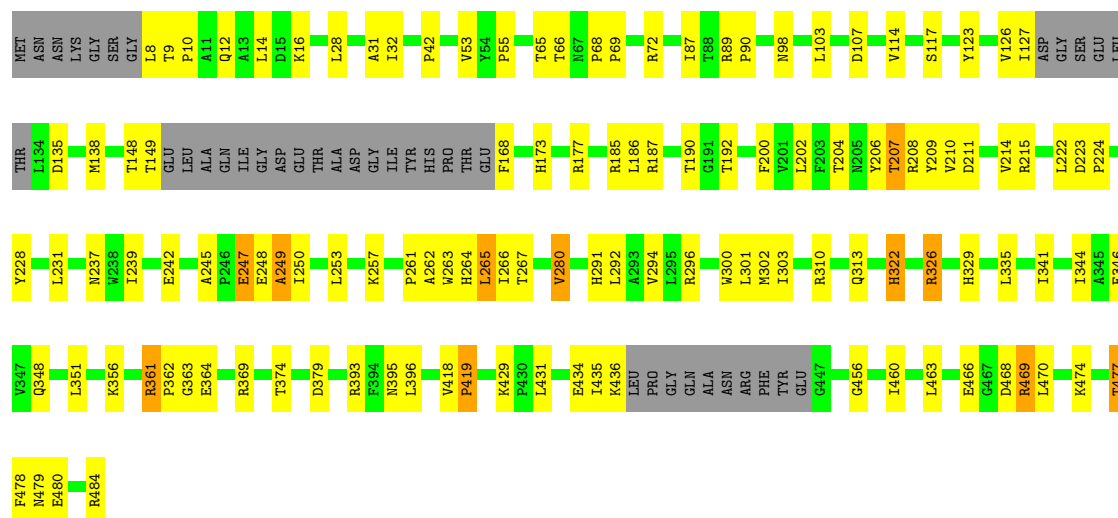
Chain E: 





• Molecule 1: AMP nucleosidase

Chain F: 66% 23% 8%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	246.24Å 246.24Å 111.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.75 – 2.60	Depositor
% Data completeness (in resolution range)	95.8 (36.75-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21455	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

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: FMP

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	0.39	0/3590	0.61	0/4884
1	B	0.38	0/3599	0.61	0/4896
1	C	0.39	0/3590	0.62	0/4884
1	D	0.40	0/3590	0.63	0/4884
1	E	0.39	0/3590	0.61	0/4884
1	F	0.38	0/3590	0.61	0/4884
All	All	0.39	0/21549	0.61	0/29316

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	3505	0	3444	130	0
1	B	3514	0	3450	143	0
1	C	3505	0	3444	124	0
1	D	3505	0	3444	102	0
1	E	3505	0	3444	119	0
1	F	3505	0	3444	109	0
2	A	23	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	23	0	11	0	0
2	C	23	0	12	0	0
2	D	23	0	11	0	0
2	E	23	0	11	0	0
2	F	23	0	11	0	0
3	A	44	0	0	3	0
3	B	43	0	0	7	0
3	C	42	0	0	3	0
3	D	71	0	0	6	0
3	E	46	0	0	3	0
3	F	32	0	0	2	0
All	All	21455	0	20737	689	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 16.

The worst 5 of 689 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:E:361:ARG:HD3	1:E:361:ARG:H	1.03	1.11
1:C:361:ARG:H	1:C:361:ARG:HD3	1.20	1.07
1:E:192:THR:HG21	1:E:264:HIS:HE2	1.20	1.06
1:F:361:ARG:H	1:F:361:ARG:HD3	1.20	1.04
1:A:435:ILE:HG22	1:A:436:LYS:H	1.24	1.03

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	435/484 (90%)	413 (95%)	15 (3%)	7 (2%)	8 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	436/484 (90%)	411 (94%)	22 (5%)	3 (1%)	19	38
1	C	435/484 (90%)	412 (95%)	19 (4%)	4 (1%)	14	31
1	D	435/484 (90%)	412 (95%)	17 (4%)	6 (1%)	9	19
1	E	435/484 (90%)	410 (94%)	21 (5%)	4 (1%)	14	31
1	F	435/484 (90%)	409 (94%)	23 (5%)	3 (1%)	19	38
All	All	2611/2904 (90%)	2467 (94%)	117 (4%)	27 (1%)	13	29

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLU
1	B	66	THR
1	C	66	THR
1	D	66	THR
1	F	66	THR

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	375/403 (93%)	350 (93%)	25 (7%)	13	29
1	B	376/403 (93%)	350 (93%)	26 (7%)	13	28
1	C	375/403 (93%)	350 (93%)	25 (7%)	13	29
1	D	375/403 (93%)	350 (93%)	25 (7%)	13	29
1	E	375/403 (93%)	350 (93%)	25 (7%)	13	29
1	F	375/403 (93%)	350 (93%)	25 (7%)	13	29
All	All	2251/2418 (93%)	2100 (93%)	151 (7%)	13	29

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	301	LEU

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Mol	Chain	Res	Type
1	F	351	LEU
1	E	361	ARG
1	F	202	LEU
1	F	477	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	284	ASN
1	F	313	GLN
1	E	322	HIS
1	F	119	HIS
1	C	12	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	FMP	F	506	-	24,25,25	1.27	4 (16%)	25,38,38	1.77	4 (16%)
2	FMP	C	503	-	24,25,25	1.30	4 (16%)	25,38,38	1.86	3 (12%)
2	FMP	D	504	-	24,25,25	1.28	4 (16%)	25,38,38	2.01	5 (20%)
2	FMP	E	505	-	24,25,25	1.26	4 (16%)	25,38,38	1.97	6 (24%)
2	FMP	A	501	-	24,25,25	1.20	5 (20%)	25,38,38	1.84	3 (12%)
2	FMP	B	502	-	24,25,25	1.26	2 (8%)	25,38,38	1.97	5 (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
2	FMP	F	506	-	-	2/6/26/26	0/3/3/3
2	FMP	C	503	-	-	2/6/26/26	0/3/3/3
2	FMP	D	504	-	-	2/6/26/26	0/3/3/3
2	FMP	E	505	-	-	1/6/26/26	0/3/3/3
2	FMP	A	501	-	-	2/6/26/26	0/3/3/3
2	FMP	B	502	-	-	2/6/26/26	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	503	FMP	C2'-C1'	-3.16	1.50	1.54
2	D	504	FMP	C2'-C1'	-2.77	1.50	1.54
2	F	506	FMP	C4-N3	2.70	1.40	1.37
2	B	502	FMP	C2'-C1'	-2.68	1.50	1.54
2	D	504	FMP	O4'-C1'	-2.60	1.40	1.44

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	504	FMP	O4'-C1'-C2'	6.83	115.88	104.56
2	B	502	FMP	O4'-C1'-C2'	6.48	115.30	104.56
2	E	505	FMP	O4'-C1'-C2'	6.23	114.88	104.56
2	A	501	FMP	O4'-C1'-C2'	5.91	114.36	104.56
2	C	503	FMP	O4'-C1'-C2'	5.72	114.04	104.56

There are no chirality outliers.

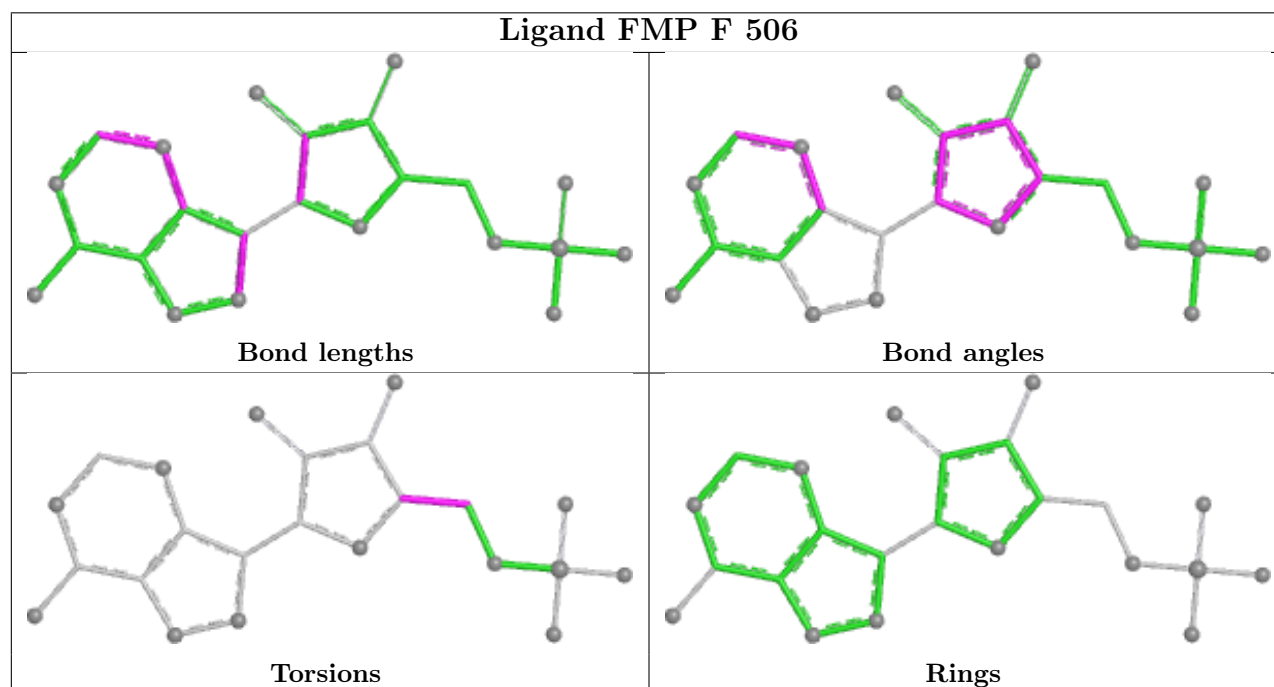
5 of 11 torsion outliers are listed below:

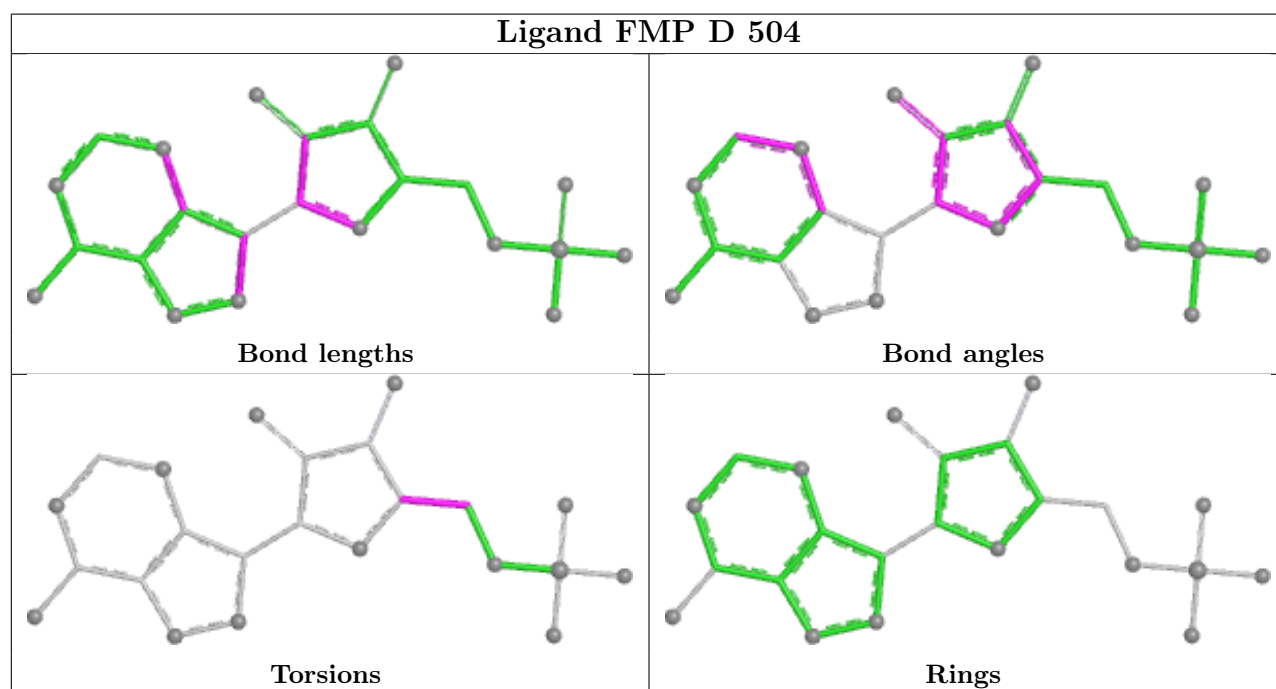
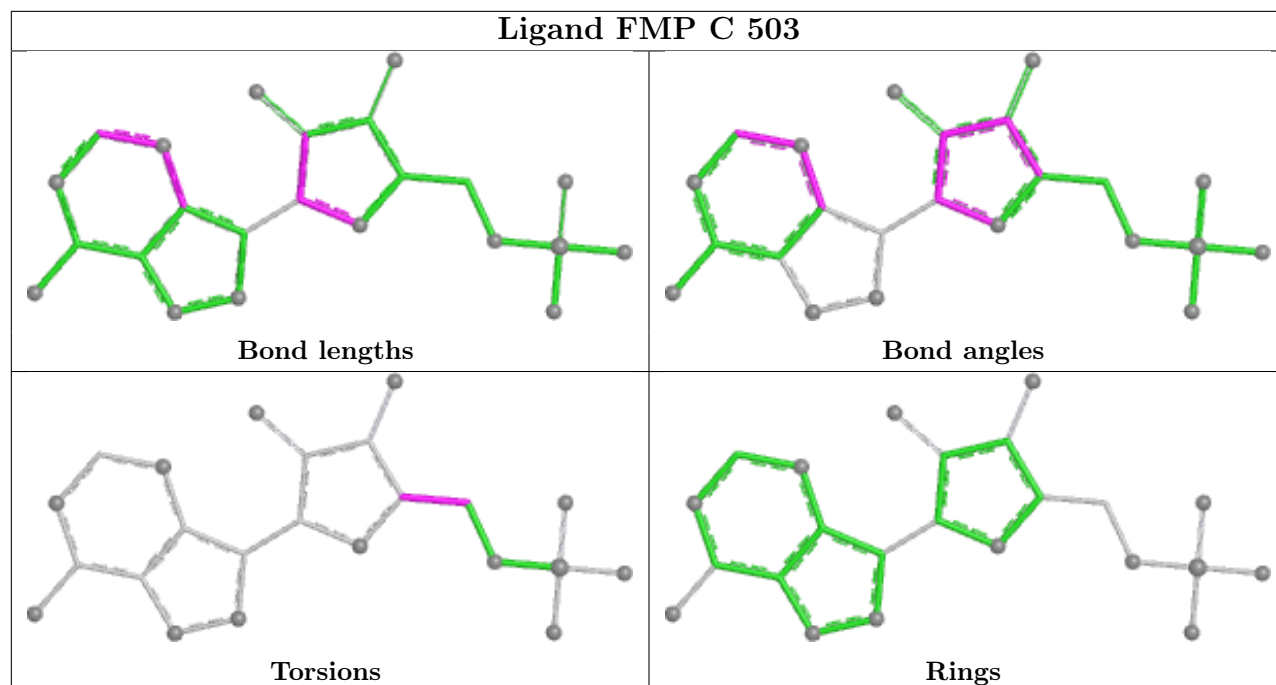
Mol	Chain	Res	Type	Atoms
2	F	506	FMP	C3'-C4'-C5'-O5'
2	D	504	FMP	C3'-C4'-C5'-O5'
2	A	501	FMP	C3'-C4'-C5'-O5'
2	B	502	FMP	C3'-C4'-C5'-O5'
2	C	503	FMP	C3'-C4'-C5'-O5'

There are no ring outliers.

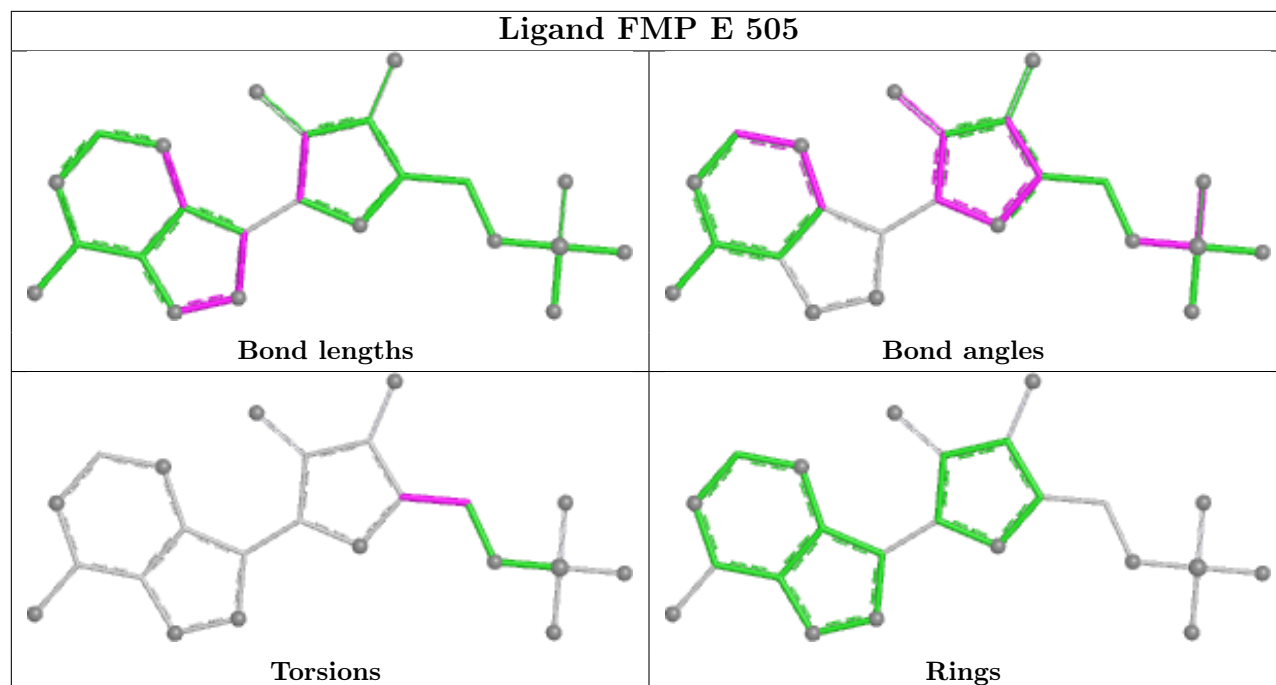
No monomer is involved in short contacts.

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.

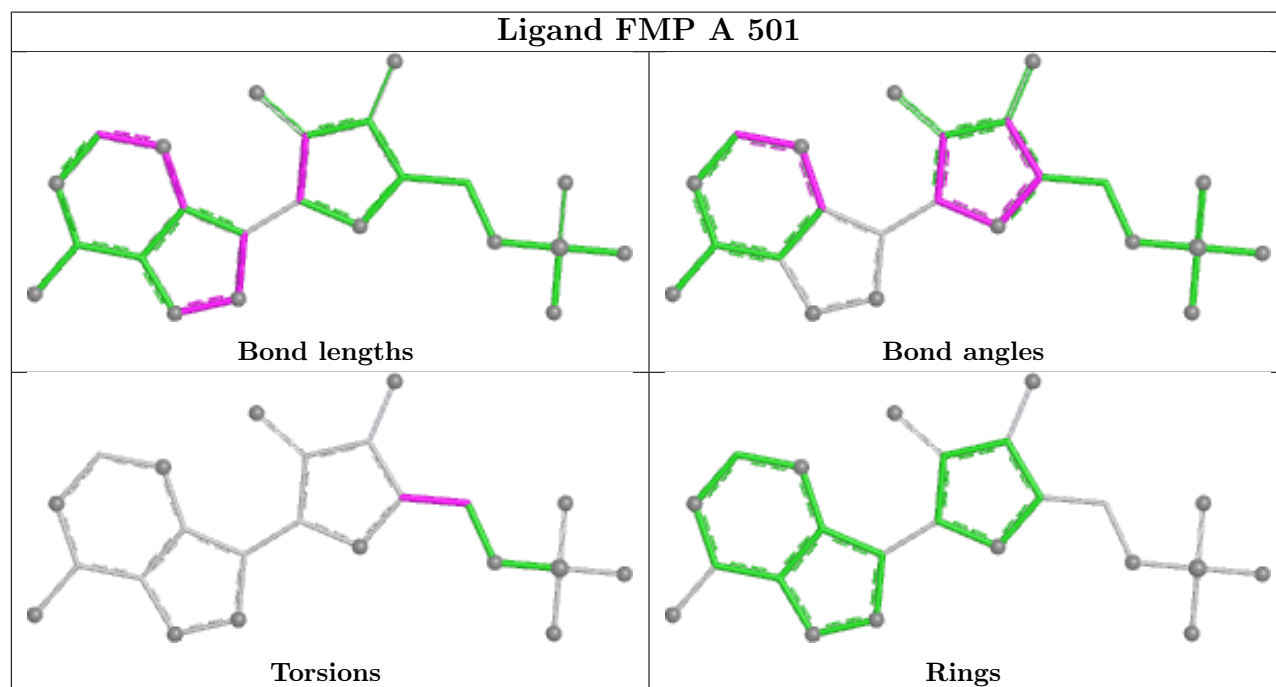


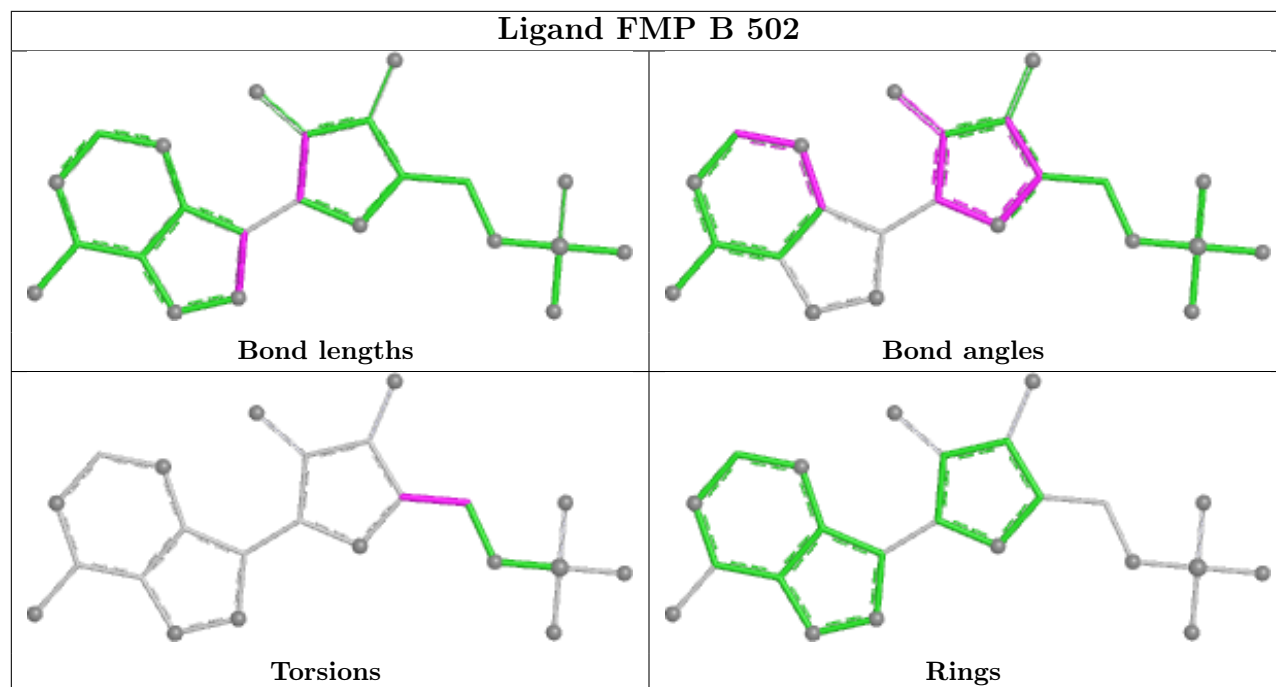


Ligand FMP E 505



Ligand FMP A 501





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.