

wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 07:19 AM EDT

PDB ID : 4IMY

Title: The AFF4 scaffold binds human P-TEFb adjacent to HIV Tat

Authors : Alber, T.; Schulze-Gahmen, U.

Deposited on : 2013-01-03

Resolution : 2.94 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 (1)) 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)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

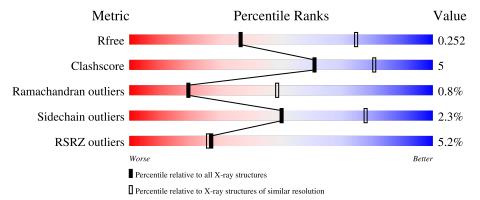
Validation Pipeline (wwPDB-VP) : 2.35.1

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 2.94 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	A	332	82%	11%	• 5%
1			4%	11 /6	• 5/0
1	С	332	82% 7%	11%	- 6%
1	E	332	81%	12%	- 5%
2	В	264	85%	9%	5%
			4%		
2	D	264	88%	7%	5%



Mol	Chain	Length		Quality of chain								
2	F	264	.%		85%			9%	6%			
3	G	75	7%	32%	12%		56%		_			
3	Н	75	8%	53%		17%		29%	_			
3	I	75	3%	36%	8%		56%					

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:

M	Iol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	4	AMP	A	401	-	-	X	X



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 29134 atoms, of which 14526 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 Cyclin-dependent kinase 9.

Mol	Chain	Residues			Ato	ms	ZeroOcc	AltConf	Trace			
1	Λ	315	Total	С	Н	N	О	Р	S	0	0	0
1	A	319	5120	1625	2585	435	459	1	15	0	0	U
1	С	311	Total	С	Н	N	О	Р	S	0	0	0
1		311	5079	1608	2569	433	453	1	15	0	0	U
1	Е	314	Total	С	Н	N	О	Р	S	0	0	0
1	15	314	5128	1626	2593	435	458	1	15	0	U	U

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P50750
A	0	HIS	-	expression tag	UNP P50750
С	-1	GLY	-	expression tag	UNP P50750
С	0	HIS	_	expression tag	UNP P50750
Е	-1	GLY	-	expression tag	UNP P50750
E	0	HIS	-	expression tag	UNP P50750

• Molecule 2 is a protein called Cyclin-T1.

Mol	Chain	Residues			Atoms	S	ZeroOcc	AltConf	Trace			
2	B	250	Total	С	Н	N	О	S	0	0	0	
2	Б	250	3974	1282	1971	342	370	9	0	U	U	
2	D	251	Total	С	Н	N	О	S	0	0	0	
2	D	251	4020	1292	1996	348	375	9	0	U	0	
2	F	249	Total	С	Н	N	О	S	0	0	0	
	I'	249	3974	1280	1973	342	370	9	0	U	U	

• Molecule 3 is a protein called AF4/FMR2 family member 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	33	Total 470	C 160	H 222	N 36	O 50	S 2	0	0	0

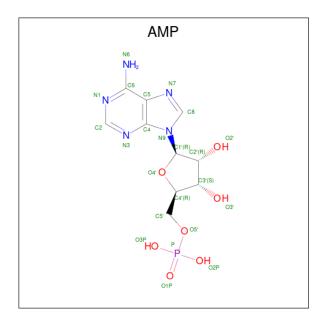


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	Н	53	Total 783	C 254				S 4	0	3	0
3	I	33	Total 462	С		N	О	S 2	0	0	0

There are 9 discrepancies between the modelled and reference sequences: $\frac{1}{2}$

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	SER	-	expression tag	UNP Q9UHB7
G	0	ASN	-	expression tag	UNP Q9UHB7
G	1	ALA	-	expression tag	UNP Q9UHB7
Н	-1	SER	-	expression tag	UNP Q9UHB7
Н	0	ASN	-	expression tag	UNP Q9UHB7
Н	1	ALA	-	expression tag	UNP Q9UHB7
I	-1	SER	-	expression tag	UNP Q9UHB7
I	0	ASN	-	expression tag	UNP Q9UHB7
I	1	ALA	-	expression tag	UNP Q9UHB7

 $\bullet \ \ Molecule\ 4\ is\ ADENOSINE\ MONOPHOSPHATE\ (three-letter\ code:\ AMP)\ (formula:\ C_{10}H_{14}N_5O_7P).$



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	٨	1	Total	С	Н	N	О	Р	0	0
4	A	1	35	10	12	5	7	1	U	U
4	С	1	Total	С	Н	N	О	Р	0	0
4		1	35	10	12	5	7	1		0



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	E	1	Total	С	Н	N	О	Р	0	0
_ T		1	35	10	12	5	7	1		

• Molecule 5 is water.

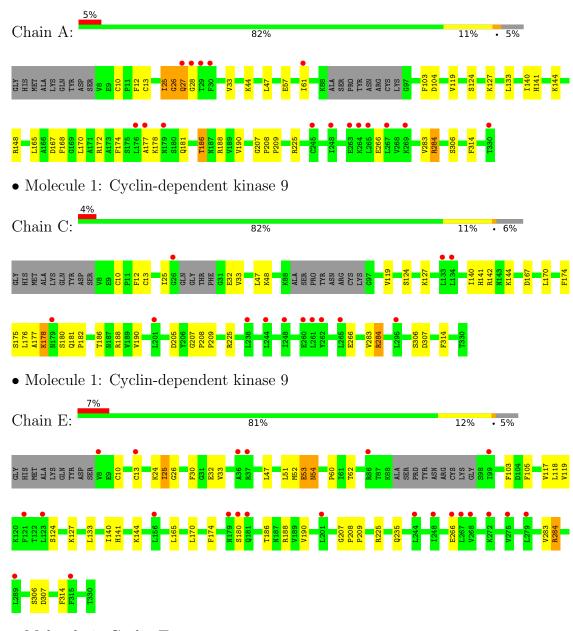
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	В	2	Total O 2 2	0	0
5	С	5	Total O 5 5	0	0
5	D	3	Total O 3 3	0	0
5	E	5	Total O 5 5	0	0
5	F	1	Total O 1 1	0	0



3 Residue-property plots (i)

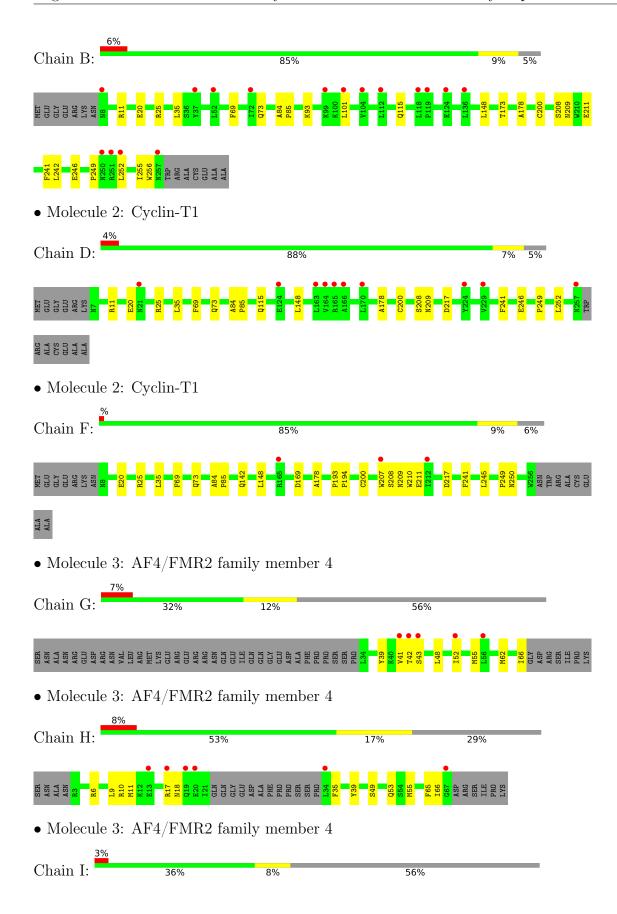
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Cyclin-dependent kinase 9



• Molecule 2: Cyclin-T1











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	100.69Å 126.30Å 195.63Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 - 2.94	Depositor
rtesolution (A)	48.76 - 2.93	EDS
% Data completeness	99.7 (48.76-2.94)	Depositor
(in resolution range)	94.7 (48.76-2.93)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	1.39 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
D D	0.207 , 0.245	Depositor
R, R_{free}	0.217 , 0.252	DCC
R_{free} test set	2000 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 76.0	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29134	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: AMP, TPO

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	Bo	nd lengths	Bond angles	
IVIOI	Moi Chain		# Z > 5	RMSZ	# Z >5
1	A	0.23	0/2574	0.40	0/3475
1	С	0.23	0/2547	0.40	0/3436
1	Е	0.23	0/2574	0.40	0/3474
2	В	0.25	0/2053	0.39	0/2801
2	D	0.32	2/2074~(0.1%)	0.39	0/2828
2	F	0.25	0/2051	0.38	0/2798
3	G	0.24	0/252	0.36	0/340
3	Н	0.22	0/424	0.38	0/566
3	I	0.23	0/246	0.37	0/330
All	All	0.25	$2/14795 \ (0.0\%)$	0.39	0/20048

All (2) bond length outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}({ ext{ iny A}})$
2	D	115	GLN	CD-NE2	-7.70	1.13	1.32
2	D	115	GLN	CD-OE1	-6.63	1.09	1.24

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	2535	2585	2578	29	1
1	С	2510	2569	2561	29	0
1	Ε	2535	2593	2586	33	1
2	В	2003	1971	1960	19	0
2	D	2024	1996	1985	9	0
2	F	2001	1973	1962	13	0
3	G	248	222	222	10	0
3	Н	421	362	354	12	0
3	I	243	219	219	7	0
4	A	23	12	12	7	0
4	С	23	12	12	2	0
4	Ε	23	12	12	2	0
5	A	3	0	0	0	0
5	В	2	0	0	1	0
5	С	5	0	0	0	0
5	D	3	0	0	0	0
5	Е	5	0	0	0	0
5	F	1	0	0	0	0
All	All	14608	14526	14463	132	1

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 5.

The worst 5 of 132 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:26:GLY:O	1:A:28:GLY:N	2.06	0.88
1:C:177:ALA:HB1	1:C:178:LYS:HG3	1.62	0.81
1:C:178:LYS:NZ	1:C:180:SER:OG	2.14	0.81
1:C:307:ASP:OD1	3:H:17:ARG:NH2	2.14	0.81
1:C:177:ALA:HB1	1:C:178:LYS:CG	2.14	0.77

All (1) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:44:LYS:NZ	1:E:307:ASP:OD2[2_554]	2.02	0.18



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	Perce	ntiles
1	A	310/332 (93%)	291 (94%)	15 (5%)	4 (1%)	12	35
1	С	304/332 (92%)	288 (95%)	14 (5%)	2 (1%)	22	52
1	E	309/332 (93%)	289 (94%)	16 (5%)	4 (1%)	12	35
2	В	248/264 (94%)	237 (96%)	10 (4%)	1 (0%)	34	64
2	D	249/264 (94%)	237 (95%)	11 (4%)	1 (0%)	34	64
2	F	247/264 (94%)	236 (96%)	10 (4%)	1 (0%)	34	64
3	G	31/75 (41%)	30 (97%)	1 (3%)	0	100	100
3	Н	52/75~(69%)	49 (94%)	2 (4%)	1 (2%)	8	26
3	I	31/75 (41%)	30 (97%)	1 (3%)	0	100	100
All	All	1781/2013 (88%)	1687 (95%)	80 (4%)	14 (1%)	19	49

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	26	GLY
1	A	190	VAL
2	В	249	PRO
1	С	190	VAL

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	Perce	ntiles
1	A	276/292 (94%)	270 (98%)	6 (2%)	52	78
1	$^{\mathrm{C}}$	274/292 (94%)	265 (97%)	9 (3%)	38	69
1	E	277/292 (95%)	269 (97%)	8 (3%)	42	73
2	В	221/239 (92%)	218 (99%)	3 (1%)	67	86
2	D	225/239 (94%)	221 (98%)	4 (2%)	59	82
2	F	222/239 (93%)	217 (98%)	5 (2%)	50	78
3	G	25/69~(36%)	25 (100%)	0	100	100
3	Н	36/69~(52%)	33 (92%)	3 (8%)	11	30
3	I	23/69 (33%)	23 (100%)	0	100	100
All	All	1579/1800 (88%)	1541 (98%)	38 (2%)	50	77

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Е	266	GLU
3	Н	11[A]	MET
1	Е	306	SER
2	F	217	ASP
3	Н	35	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	232	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)

3 non-standard protein/DNA/RNA residues 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	Trme	Chain	Res	Link	Bond lengths			В	ond ang	les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	С	186	1	8,10,11	1.17	0	10,14,16	1.53	1 (10%)
1	TPO	A	186	1	8,10,11	1.13	0	10,14,16	1.26	2 (20%)
1	TPO	Е	186	1	8,10,11	1.13	0	10,14,16	1.12	0

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
1	TPO	С	186	1	-	0/9/11/13	-
1	TPO	A	186	1	-	4/9/11/13	-
1	TPO	E	186	1	-	5/9/11/13	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
1	С	186	TPO	P-OG1-CB	-4.10	110.82	123.21
1	A	186	TPO	P-OG1-CB	-2.49	115.68	123.21
1	A	186	TPO	CG2-CB-CA	-2.11	109.01	113.16

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	186	TPO	N-CA-CB-CG2
1	A	186	TPO	N-CA-CB-OG1
1	A	186	TPO	C-CA-CB-CG2
1	A	186	TPO	CG2-CB-OG1-P
1	Е	186	TPO	N-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

	Mol	Chain	Res	Type	Clashes	Symm-Clashes
ſ	1	A	186	TPO	1	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	186	TPO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	Tune	Chain	Res	Link	Вс	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AMP	С	401	-	22,25,25	0.91	2 (9%)	25,38,38	1.37	3 (12%)
4	AMP	A	401	-	22,25,25	0.86	1 (4%)	25,38,38	1.19	2 (8%)
4	AMP	Е	401	-	22,25,25	0.86	1 (4%)	25,38,38	1.23	2 (8%)

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	AMP	С	401	-	-	3/6/26/26	0/3/3/3
4	AMP	A	401	-	-	1/6/26/26	0/3/3/3
4	AMP	Ε	401	-	-	0/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
4	С	401	AMP	C5-C4	2.37	1.47	1.40
4	Е	401	AMP	C5-C4	2.30	1.47	1.40
4	A	401	AMP	C5-C4	2.25	1.46	1.40
4	С	401	AMP	C2-N3	2.05	1.35	1.32



The worst	5	of	7	bond	angle	outliers	are	listed	below:
111 0 110100	$\overline{}$	O.	•	OIL	WII 510	OGGIICID	COL C	IID CCC	OCIO III.

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
4	С	401	AMP	N3-C2-N1	-3.66	122.96	128.68
4	Е	401	AMP	N3-C2-N1	-3.66	122.96	128.68
4	A	401	AMP	N3-C2-N1	-3.63	123.01	128.68
4	С	401	AMP	O2'-C2'-C3'	2.40	119.58	111.82
4	Е	401	AMP	C4-C5-N7	-2.28	107.03	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	С	401	AMP	C5'-O5'-P-O2P
4	С	401	AMP	C5'-O5'-P-O1P
4	A	401	AMP	C5'-O5'-P-O2P
4	С	401	AMP	C5'-O5'-P-O3P

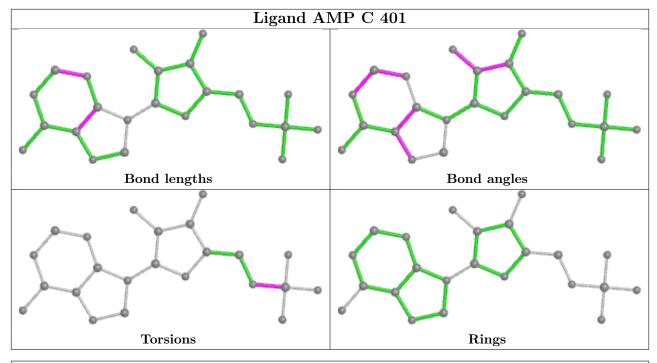
There are no ring outliers.

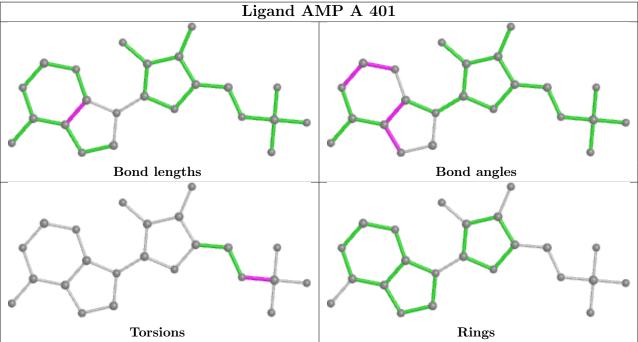
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	401	AMP	2	0
4	A	401	AMP	7	0
4	Е	401	AMP	2	0

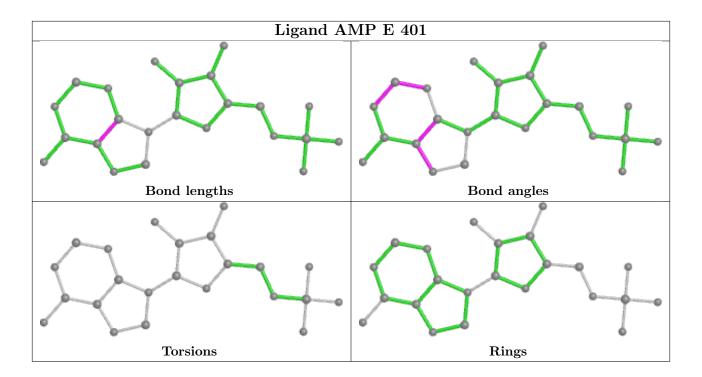
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$ullet$ Analysed $ullet$ $\langle RSRZ angle ullet$ $\#RSRZ angle 2$		$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9	
1	A	314/332~(94%)	0.52	16 (5%) 28	27	75, 99, 196, 266	0
1	С	310/332~(93%)	0.32	13 (4%) 36	35	76, 106, 183, 227	0
1	E	313/332~(94%)	0.54	23 (7%) 15	13	70, 112, 188, 246	0
2	В	250/264~(94%)	0.52	16 (6%) 19	17	77, 112, 191, 228	0
2	D	$251/264\ (95\%)$	0.44	10 (3%) 38	37	70, 116, 185, 241	0
2	F	249/264~(94%)	0.36	3 (1%) 79	80	79, 111, 169, 214	0
3	G	33/75~(44%)	0.65	5 (15%) 2	1	98, 152, 212, 237	0
3	Н	53/75~(70%)	0.53	6 (11%) 5	4	115, 164, 213, 232	0
3	I	33/75~(44%)	0.12	2 (6%) 21	19	116, 156, 206, 208	0
All	All	1806/2013 (89%)	0.45	94 (5%) 27	26	70, 111, 193, 266	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	THR	10.4
1	С	248	ILE	6.4
1	A	29	THR	5.6
1	A	28	GLY	5.2
1	С	179	ASN	5.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	TPO	Е	186	11/12	0.92	0.24	110,124,152,177	0
1	TPO	С	186	11/12	0.93	0.19	92,106,125,130	0
1	TPO	A	186	11/12	0.96	0.18	106,118,141,146	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

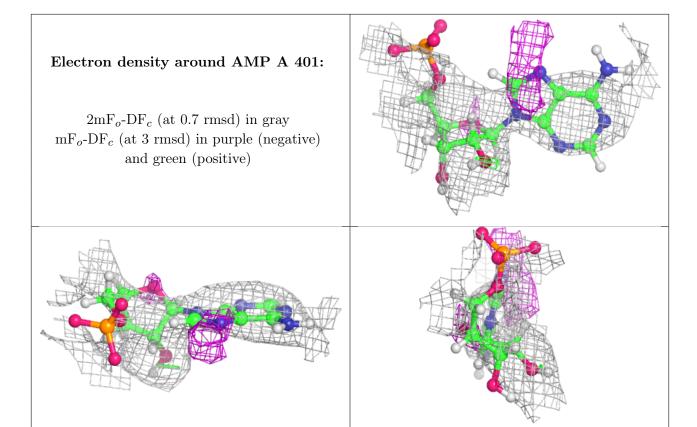
6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
4	AMP	A	401	23/23	0.75	0.47	111,153,371,371	0
4	AMP	С	401	23/23	0.75	0.37	112,157,206,211	0
4	AMP	Е	401	23/23	0.76	0.35	124,160,241,245	0

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.

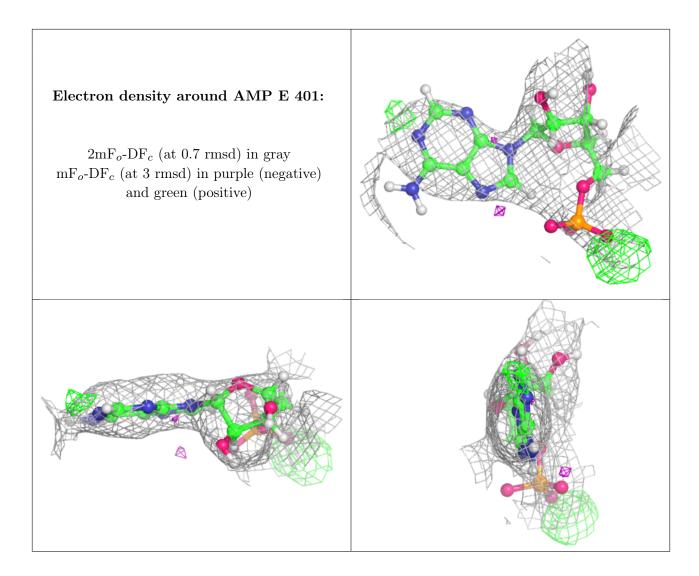






Electron density around AMP C 401: $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.

