wwPDB X-ray Structure Validation Summary Report (i)

Aug 2, 2023 – 02:26 AM EDT

PDB ID	:	1B7Y
Title	:	PHENYLALANYL TRNA SYNTHETASE COMPLEXED WITH PHENYL ALANINYL-ADENYLATE
Authors	:	Reshetnikova, L.; Moor, N.; Lavrik, O.; Vassylyev, D.G.
Deposited on	:	1999-01-26
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 (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:

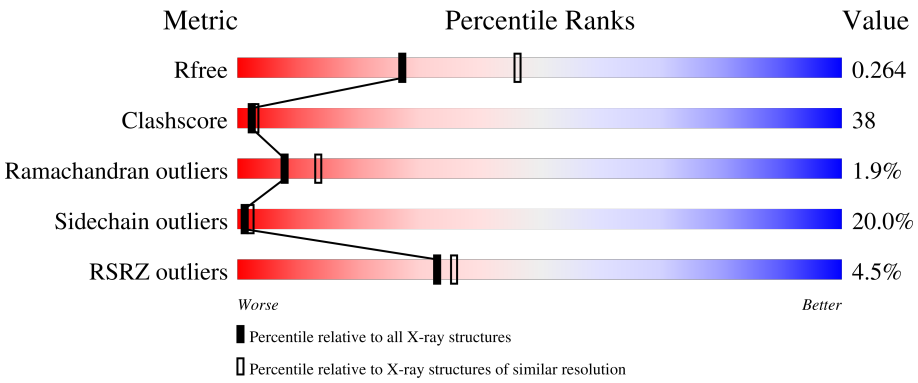
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.50 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))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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	350	2%; 33%, 34%, 9%, 24%
2	B	785	5%; 43%, 43%, 12%, ••

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8439 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 PROTEIN (PHENYLALANYL-TRNA SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	2112	1382	359	364	7	0	0	0

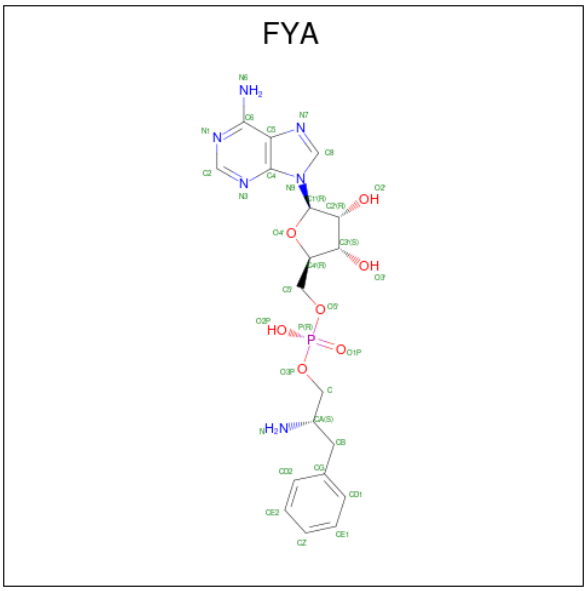
- Molecule 2 is a protein called PROTEIN (PHENYLALANYL-TRNA SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	775	6054	3879	1078	1087	10	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0

- Molecule 4 is ADENOSINE-5'-[PHENYLALANINOL-PHOSPHATE] (three-letter code: FYA) (formula: $C_{19}H_{25}N_6O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	33	19	6	7	1	0	0

- Molecule 5 is water.

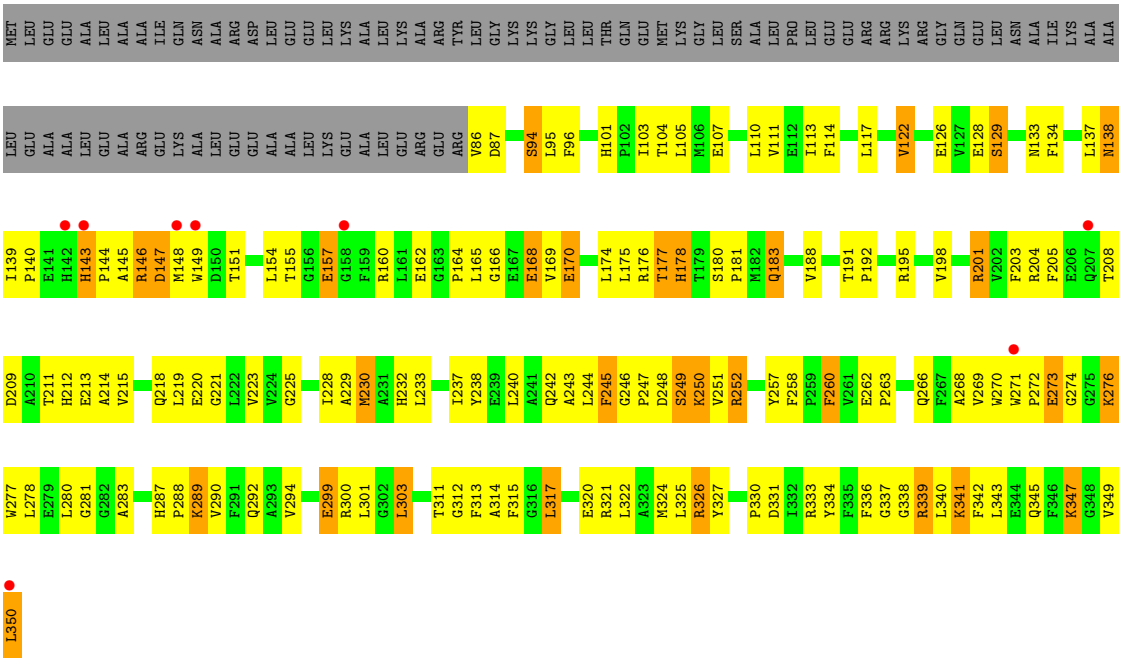
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	48	48	48	0	0
			Total	O		
5	B	191	191	191	0	0

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.

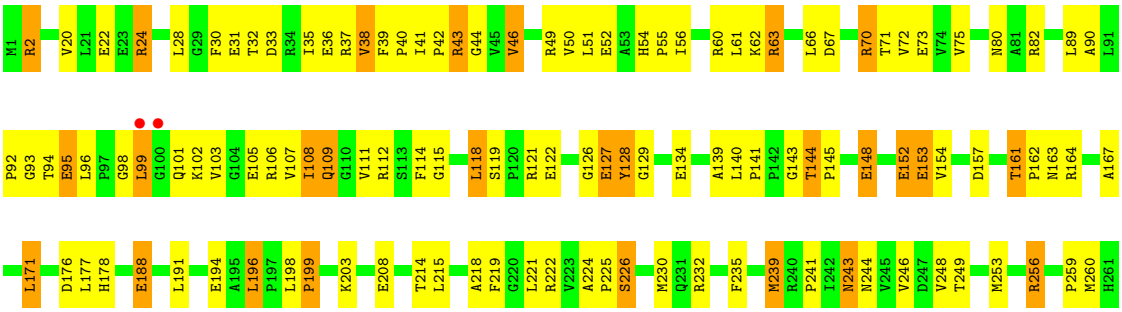
• Molecule 1: PROTEIN (PHENYLALANYL-TRNA SYNTHETASE)

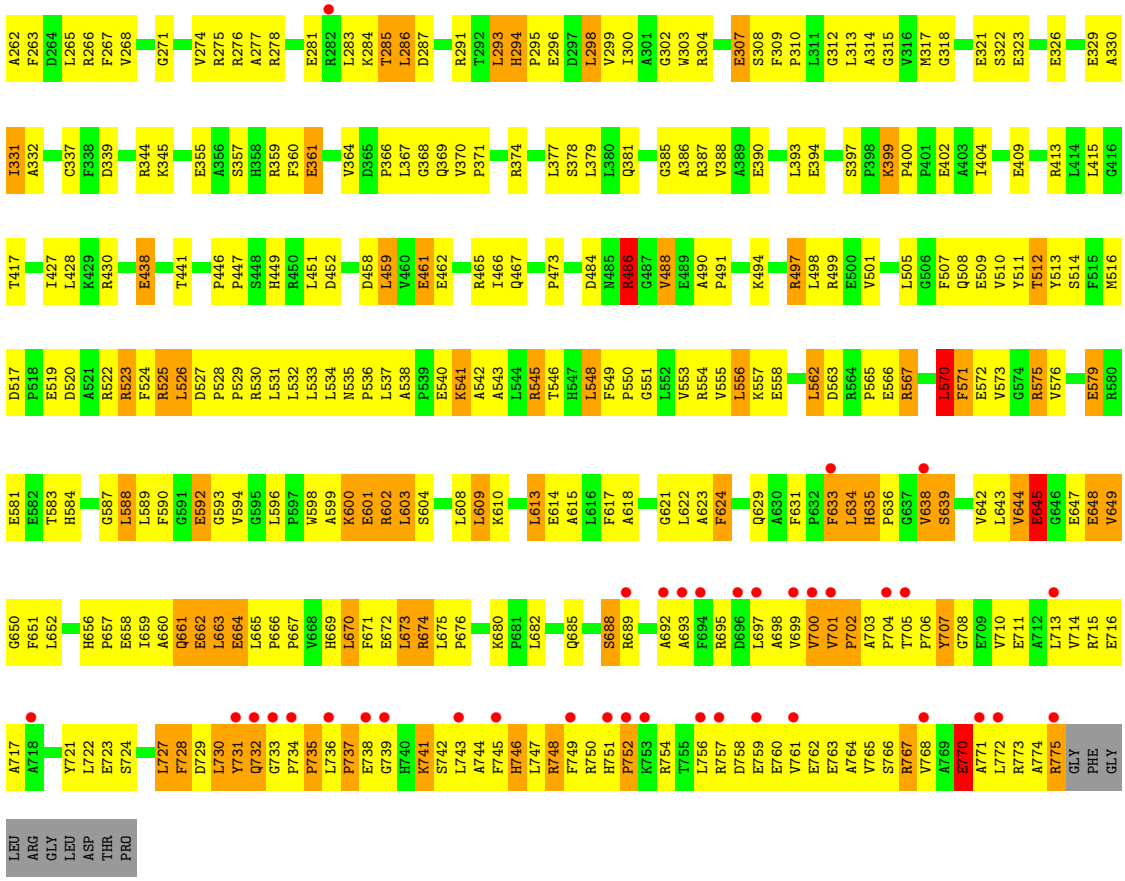
Chain A: 2% 33% 34% 9% 24%



• Molecule 2: PROTEIN (PHENYLALANYL-TRNA SYNTHETASE)

Chain B: 5% 43% 43% 12%




A262 F263 D264 L265 R266 F267 V268 G271 V274 R275 R276 A277 R278 E281 R282 L283 K284 T285 L286 D287 R291 T292 L293 H294 P295 E296 D297 L298 V299 I300 A301 G302 W303 R304 E307 S308 F309 P310 L311 G312 L313 A314 G315 V316 M317 G318 E321 S322 E323 E326 E329 A330
I331 A332 C337 F338 D339 R344 K345 E355 A356 S357 H358 R359 F360 E361 V364 D365 P366 L367 G368 Q369 V370 P371 R374 L377 S378 L379 L380 Q381 G385 A386 R387 V388 A389 E390 L393 E394 S397 P398 K399 P400 P401 E402 A403 I404 E409 R413 L414 L415 G416
T417 I427 L428 K429 R430 E438 T441 P446 P447 S448 H449 R450 L451 D452 D458 L459 V460 E461 E462 R465 I466 Q467 P473 D484 N485 R486 G487 V488 E489 A490 P491 K494 R497 L498 R499 E500 V501 L505 G506 F507 Q508 E509 V510 Y511 T512 Y513 S514 F515 M516
D517 P518 E519 D520 A521 R522 R523 F524 R525 L526 D527 P528 P529 R530 L531 L532 L533 L534 N535 P536 L537 A538 P539 E540 K541 A542 A543 L544 R545 T546 H547 L548 F549 P550 G551 L552 V553 R554 V555 L556 K557 E558 L562 D563 R564 P565 E566 R567 L570 F571 E572 V573 G574 R575 V576 E579 R580
E581 E582 T583 H584 G587 L588 L589 F590 G591 E592 G593 V594 G595 L596 P597 W598 A599 K600 E601 R602 L603 S604 L608 L609 K610 L613 E614 A615 L616 F617 A618 G621 L622 A623 F624 Q629 A630 F631 P632 F633 L634 H635 P636 G637 V638 S639 V642 L643 V644 E645 G646 E647 E648 V649
G650 F651 L652 H656 P657 E658 I659 A660 Q661 E662 L663 E664 L665 P666 P667 V668 H669 L670 F671 E672 L673 R674 L675 P676 K680 P681 L682 Q685 S688 R689 A692 A693 F694 R695 D696 L697 A698 V699 V700 V701 P702 A703 P704 T705 P706 Y707 G708 E709 V710 E711 A712 L713 V714 R715 E716
A717 A718 Y721 L722 E723 S724 L727 F728 D729 L730 Q731 Q732 G733 P734 P735 L736 P737 E738 G739 H740 K741 S742 L743 A744 F745 H746 L747 R748 F749 R750 H751 P752 K753 R754 T755 L756 R757 D758 E759 E760 V761 E762 E763 A764 V765 S766 R767 V768 A769 E770 A771 L772 R773 A774 R775 GLY PHE GLY
LEU ARG GLY LEU ASP THR PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.50Å 174.50Å 140.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 47.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.50) 95.7 (47.41-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	15112.19 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.230 , 0.267 0.229 , 0.264	Depositor DCC
R_{free} test set	4109 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 82.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8439	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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.

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: FYA, 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	0.54	0/2180	0.76	0/2957
2	B	0.53	0/6205	0.79	4/8436 (0.0%)
All	All	0.53	0/8385	0.78	4/11393 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	115	GLY	N-CA-C	-5.83	98.54	113.10
2	B	601	GLU	CB-CA-C	-5.59	99.22	110.40
2	B	128	TYR	N-CA-C	5.35	125.44	111.00
2	B	570	LEU	CA-CB-CG	5.28	127.44	115.30

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	2112	0	2062	164	0
2	B	6054	0	6109	495	0
3	A	1	0	0	0	0
4	A	33	0	24	4	0
5	A	48	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	191	0	0	6	0
All	All	8439	0	8195	626	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 38.

The worst 5 of 626 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:A:262:GLU:HG2	5:A:1015:HOH:O	1.45	1.16
2:B:600:LYS:HG2	2:B:601:GLU:H	1.04	1.14
2:B:75:VAL:HG11	2:B:108:ILE:HG21	1.31	1.12
2:B:285:THR:HG21	2:B:291:ARG:HE	1.20	1.02
2:B:294:HIS:CD2	2:B:296:GLU:H	1.79	1.00

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	263/350 (75%)	244 (93%)	14 (5%)	5 (2%)	8 13
2	B	773/785 (98%)	695 (90%)	63 (8%)	15 (2%)	8 13
All	All	1036/1135 (91%)	939 (91%)	77 (7%)	20 (2%)	8 13

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
2	B	488	VAL
2	B	664	GLU

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Mol	Chain	Res	Type
1	A	338	GLY
2	B	708	GLY

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	213/277 (77%)	176 (83%)	37 (17%)	2 3
2	B	623/630 (99%)	493 (79%)	130 (21%)	1 2
All	All	836/907 (92%)	669 (80%)	167 (20%)	1 2

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	558	GLU
2	B	673	LEU
2	B	571	PHE
2	B	624	PHE
2	B	701	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	243	ASN
2	B	294	HIS
2	B	261	HIS
2	B	350	HIS
1	A	218	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	FYA	A	1002	-	33,36,36	1.22	3 (9%)	35,52,52	0.84	1 (2%)

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	FYA	A	1002	-	-	5/16/36/36	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	FYA	O3P-C	-4.45	1.27	1.44
4	A	1002	FYA	O4'-C1'	2.63	1.44	1.41
4	A	1002	FYA	C8-N7	-2.12	1.30	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1002	FYA	C3'-C2'-C1'	2.76	105.13	100.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	FYA	O3P-C-CA-N
4	A	1002	FYA	O3P-C-CA-CB
4	A	1002	FYA	C-CA-CB-CG
4	A	1002	FYA	N-CA-CB-CG
4	A	1002	FYA	C5'-O5'-P-O3P

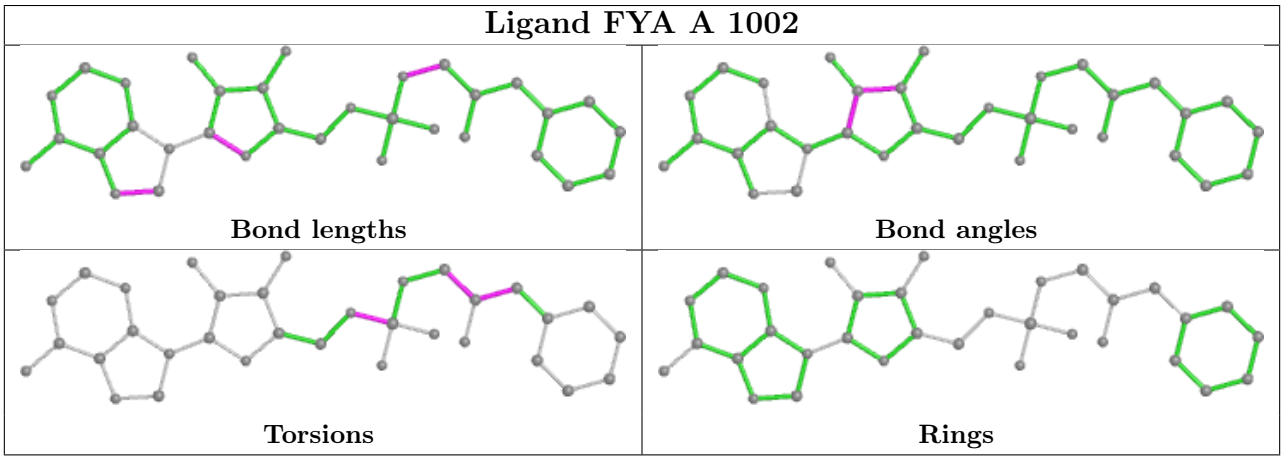
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	FYA	4	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 FYA A 1002



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, 95th 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	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	265/350 (75%)	0.06	8 (3%)	50	53	27, 54, 103, 129	0
2	B	775/785 (98%)	0.08	39 (5%)	28	30	21, 59, 108, 128	0
All	All	1040/1135 (91%)	0.08	47 (4%)	33	36	21, 58, 107, 129	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	TRP	5.6
2	B	718	ALA	5.0
1	A	350	LEU	4.9
2	B	753	LYS	4.8
2	B	739	GLY	4.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

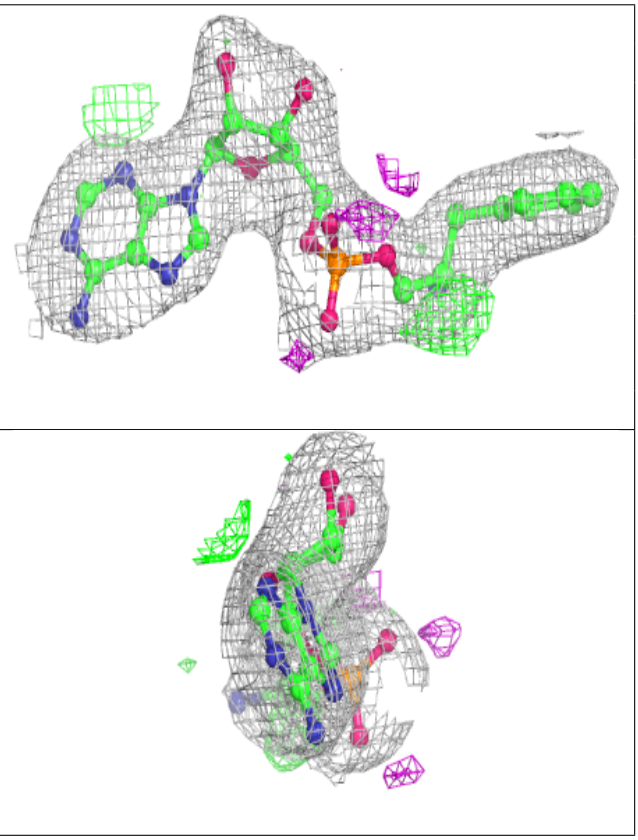
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	1001	1/1	0.85	0.26	42,42,42,42	0
4	FYA	A	1002	33/33	0.97	0.15	40,65,73,76	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 FYA A 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.