

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 12:01 PM EDT

PDB ID : 1A5A

Title: CRYO-CRYSTALLOGRAPHY OF A TRUE SUBSTRATE, INDOLE-3-

GLYCEROL PHOSPHATE, BOUND TO A MUTANT (ALPHAD60N) TRYPTOPHAN SYNTHASE ALPHA2BETA2 COMPLEX REVEALS THE

CORRECT ORIENTATION OF ACTIVE SITE ALPHA GLU 49

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Deposited on : 1998-02-12

Resolution : 1.90 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 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 : 2.23.2

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)

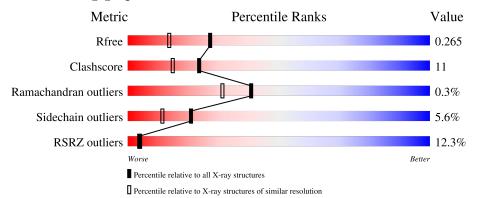
Validation Pipeline (wwPDB-VP) : 2.23.2

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 1.90 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	268	71%	22%	• 5%
2	В	397	73%	23%	



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5289 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 TRYPTOPHAN SYNTHASE (ALPHA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	255	Total	С	N	О	S	0	0	0
1	Λ	255	1929	1230	333	358	8	U	U	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASN	ASP	engineered mutation	UNP P00929

• Molecule 2 is a protein called TRYPTOPHAN SYNTHASE (BETA CHAIN).

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
2	В	389	Total 2950	C 1855	N 518	O 558	S 19	0	0	0

There is a discrepancy between the modelled and reference sequences:

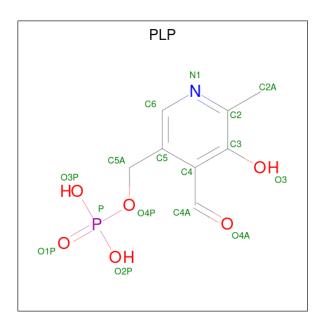
Chain	Residue	Modelled	Actual	Comment	Reference
В	396	LEU	GLU	conflict	UNP P0A2K1

• Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total K 1 1	0	0

• Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
1	D	1	Total	С	N	О	Р	0	0
4	Б	1	15	8	1	5	1	0	U

• Molecule 5 is water.

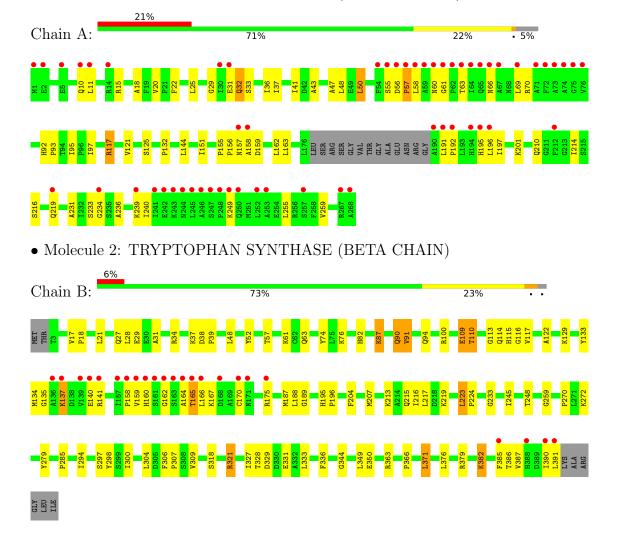
\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	120	Total O 120 120	0	0
5	В	274	Total O 274 274	0	0



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: TRYPTOPHAN SYNTHASE (ALPHA CHAIN)





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	183.50Å 59.40Å 67.30Å	Donositor
a, b, c, α , β , γ	90.00° 94.60° 90.00°	Depositor
Resolution (Å)	8.00 - 1.90	Depositor
Resolution (A)	8.00 - 1.90	EDS
% Data completeness	77.7 (8.00-1.90)	Depositor
(in resolution range)	83.6 (8.00-1.90)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	2.13 (at 1.90Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
D D	0.238 , 0.298	Depositor
R, R_{free}	0.217 , 0.265	DCC
R_{free} test set	4911 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.736	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.50 , 104.3	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5289	wwPDB-VP
Average B, all atoms $(Å^2)$	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.18% 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: PLP, K

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	Boı	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.36	0/1968	0.61	0/2673	
2	В	0.42	1/3008~(0.0%)	0.68	0/4064	
All	All	0.40	1/4976~(0.0%)	0.65	0/6737	

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
2	В	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
2	В	87	LYS	CB-CG	6.14	1.69	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	298	TYR	Sidechain

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1929	0	1940	38	0
2	В	2950	0	2924	75	0
3	В	1	0	0	0	0
4	В	15	0	7	0	0
5	A	120	0	0	1	0
5	В	274	0	0	17	0
All	All	5289	0	4871	109	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 11.

The worst 5 of 109 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:A:57:PRO:HB2	1:A:60:ASN:HB2	1.37	1.03
1:A:56:ASP:HB2	2:B:167:LYS:HE2	1.59	0.84
2:B:90:GLN:HE22	2:B:94:GLN:HE21	1.25	0.82
2:B:135:GLY:HA2	2:B:159:VAL:HG12	1.66	0.78
2:B:166:LEU:HA	5:B:777:HOH:O	1.86	0.75

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	Percen	tiles
1	A	$251/268 \; (94\%)$	242 (96%)	7 (3%)	2 (1%)	19	9
2	В	387/397 (98%)	371 (96%)	16 (4%)	0	100	100
All	All	638/665~(96%)	613 (96%)	23 (4%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	55	SER
1	A	57	PRO

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	otameric Outliers		Percentiles		
1	A	199/208 (96%)	188 (94%)	11 (6%)	21	12		
2	В	305/311 (98%)	288 (94%)	17 (6%)	21	11		
All	All	504/519 (97%)	476 (94%)	28 (6%)	21	11		

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	109	GLU
2	В	391	LEU
2	В	140	GLU
2	В	371	LEU
2	В	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	В	145	ASN
2	В	195	HIS
2	В	365	GLN
1	A	210	GLN
2	В	27	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).

Mo	1 Type	Chain	Dog	Link	Bo	nd leng	ths	В	ond ang	les
IVIC	Type	Cham	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PLP	В	501	2	15,15,16	4.01	9 (60%)	20,22,23	2.19	5 (25%)

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	\mathbf{Type}	Chain	Res	Link	Chirals	Torsions	Rings
4	PLP	В	501	2	-	0/6/6/8	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
4	В	501	PLP	C3-C4	9.24	1.59	1.40
4	В	501	PLP	C4A-C4	6.35	1.64	1.51
4	В	501	PLP	C5-C4	4.94	1.46	1.40
4	В	501	PLP	C2-N1	4.34	1.42	1.33
4	В	501	PLP	P-O3P	-4.07	1.39	1.54

All (5) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
4	В	501	PLP	O3P-P-O4P	5.34	120.94	106.73
4	В	501	PLP	C2A-C2-C3	4.25	126.14	120.89
4	В	501	PLP	C6-N1-C2	3.93	126.45	119.17
4	В	501	PLP	O4P-C5A-C5	3.51	116.05	109.35
4	В	501	PLP	C3-C2-N1	-2.99	116.91	120.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	255/268~(95%)	1.02	56 (21%) 0 0	10, 29, 79, 94	4 (1%)
2	В	389/397 (97%)	0.13	23 (5%) 22 25	6, 17, 52, 78	3 (0%)
All	All	644/665~(96%)	0.48	79 (12%) 4 4	6, 21, 66, 94	7 (1%)

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	ALA	14.0
1	A	57	PRO	9.1
1	A	58	LEU	8.1
1	A	191	LEU	7.8
2	В	163	SER	7.7

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, 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
3	K	В	500	1/1	0.96	0.42	8,8,8,8	0
4	PLP	В	501	15/16	0.96	0.10	10,17,23,25	0

6.5 Other polymers (i)

There are no such residues in this entry.

