wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2023 – 03:11 PM EDT

PDB ID	:	3QBC
Title	:	Structure and design of a new pterin site inhibitor of S. aureus HPPK
Authors	:	Peat, T.S.; Chhabra, S.; Swarbrick, J.D.
Deposited on	:	2011-01-12
Resolution	:	1.65 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:

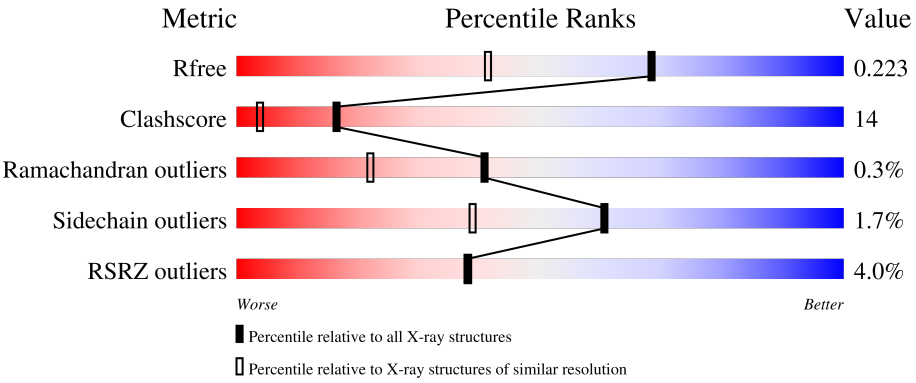
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

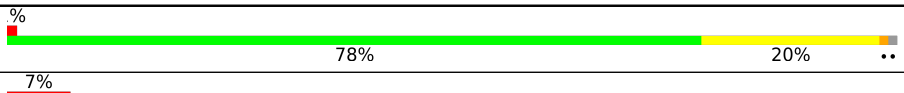
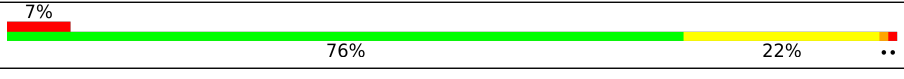
The reported resolution of this entry is 1.65 Å.

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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	161	
1	B	161	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3009 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.

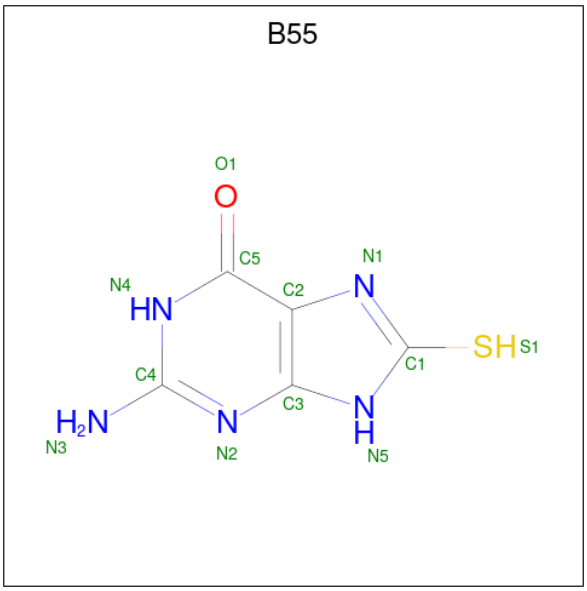
- Molecule 1 is a protein called 2-amino-4-hydroxy-6-hydroxymethyldihydropteridine pyrophosphokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	10	0
			1349	859	228	254	8			
1	B	161	Total	C	N	O	S	0	14	0
			1382	880	233	260	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q99W87
A	-1	SER	-	expression tag	UNP Q99W87
A	0	HIS	-	expression tag	UNP Q99W87
B	-2	GLY	-	expression tag	UNP Q99W87
B	-1	SER	-	expression tag	UNP Q99W87
B	0	HIS	-	expression tag	UNP Q99W87

- Molecule 2 is 2-amino-8-sulfanyl-1,9-dihydro-6H-purin-6-one (three-letter code: B55) (formula: $C_5H_5N_5OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	5	5	1	1		
2	B	1	Total	C	N	O	S	0	0
			12	5	5	1	1		

- Molecule 3 is water.

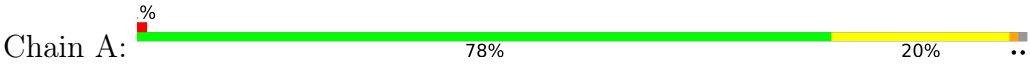
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		
3	B	127	Total	O	0	0
			127	127		

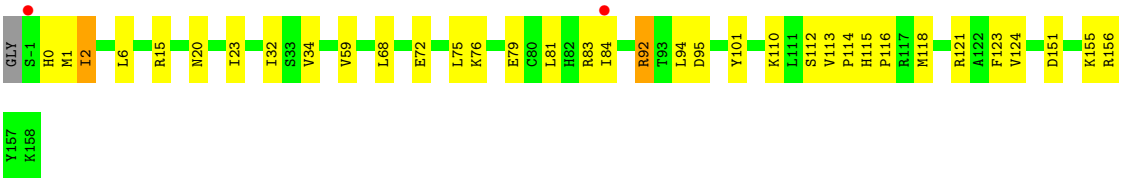
3 Residue-property plots (i)

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: 2-amino-4-hydroxy-6-hydroxymethyldihydropteridine pyrophosphokinase

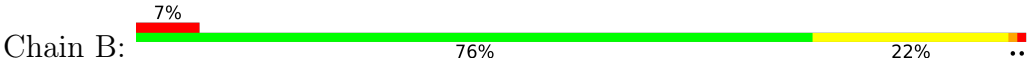
Chain A:

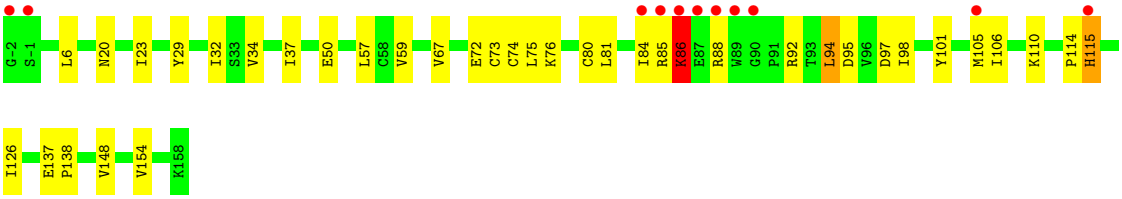




• Molecule 1: 2-amino-4-hydroxy-6-hydroxymethyldihydropteridine pyrophosphokinase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	36.79Å 76.57Å 51.52Å 90.00° 100.17° 90.00°	Depositor
Resolution (Å)	42.30 – 1.65 38.28 – 1.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.30-1.65) 100.0 (38.28-1.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.78 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.179 , 0.225 0.177 , 0.223	Depositor DCC
R_{free} test set	1684 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	11.6	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3009	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B55

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	1.11	0/1380	1.16	6/1869 (0.3%)
1	B	1.09	3/1416 (0.2%)	1.04	1/1918 (0.1%)
All	All	1.10	3/2796 (0.1%)	1.10	7/3787 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	TYR	CE1-CZ	5.36	1.45	1.38
1	B	80	CYS	CB-SG	-5.36	1.73	1.81
1	B	74	CYS	CB-SG	5.18	1.91	1.82

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	ARG	NE-CZ-NH1	11.19	125.89	120.30
1	A	92	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	15	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	94	LEU	CA-CB-CG	-6.12	101.21	115.30
1	A	156	ARG	NE-CZ-NH1	-5.76	117.42	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1349	0	1391	28	1
1	B	1382	0	1426	60	1
2	A	12	0	5	0	0
2	B	12	0	5	0	0
3	A	127	0	0	3	0
3	B	127	0	0	5	0
All	All	3009	0	2827	80	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 14.

The worst 5 of 80 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:B:20:ASN:HB2	3:B:243:HOH:O	1.33	1.26
1:A:75[B]:LEU:HD11	1:B:75:LEU:HD12	1.31	1.10
1:A:75[B]:LEU:CD1	1:B:75:LEU:CD1	2.40	1.00
1:B:86[B]:LYS:NZ	1:B:88:ARG:CZ	2.27	0.97
1:A:95[A]:ASP:OD1	1:B:110:LYS:HE3	1.71	0.90

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASN:OD1	1:B:50:GLU:OE2[2_545]	1.67	0.53

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	168/161 (104%)	165 (98%)	3 (2%)	0	100 100
1	B	173/161 (108%)	169 (98%)	2 (1%)	2 (1%)	13 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	341/322 (106%)	334 (98%)	5 (2%)	2 (1%)	41 8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	86[A]	LYS
1	B	86[B]	LYS

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	157/147 (107%)	154 (98%)	3 (2%)	57 34
1	B	161/147 (110%)	157 (98%)	4 (2%)	47 22
All	All	318/294 (108%)	311 (98%)	7 (2%)	60 27

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	ILE
1	B	86[A]	LYS
1	B	115	HIS
1	B	86[B]	LYS
1	A	84	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	62	GLN
1	B	115	HIS
1	A	3	GLN
1	A	0	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 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	B55	A	159	-	7,13,13	0.69	0	7,19,19	2.12	2 (28%)
2	B55	B	163	-	7,13,13	1.15	1 (14%)	7,19,19	1.63	1 (14%)

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	B55	A	159	-	-	-	0/2/2/2
2	B55	B	163	-	-	-	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	163	B55	C5-N4	2.47	1.41	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	159	B55	O1-C5-N4	4.48	125.94	120.65
2	B	163	B55	O1-C5-N4	3.98	125.35	120.65
2	A	159	B55	C2-C5-N4	-3.01	108.63	113.95

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

6.1 Protein, DNA and RNA chains

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>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	160/161 (99%)	-0.15	2 (1%)	77	80	4, 11, 23, 30	16 (10%)
1	B	161/161 (100%)	0.09	11 (6%)	17	16	5, 13, 30, 38	20 (12%)
All	All	321/322 (99%)	-0.03	13 (4%)	38	38	4, 12, 28, 38	36 (11%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	89	TRP	4.9
1	B	115	HIS	4.2
1	B	86[A]	LYS	3.5
1	B	84	ILE	3.1
1	B	-2	GLY	2.9

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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	B-factors(Å^2)	Q<0.9
2	B55	A	159	12/12	0.98	0.07	4,5,8,13	0
2	B55	B	163	12/12	0.98	0.07	4,6,9,10	0

6.5 Other polymers (i)

There are no such residues in this entry.