



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1SK8
Title : Crystallographic snapshots of *Aspergillus fumigatus* phytase revealing its enzymatic dynamics
Authors : Liu, Q.; Huang, Q.Q.; Lei, X.G.; Hao, Q.
Deposited on : 2004-03-04
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

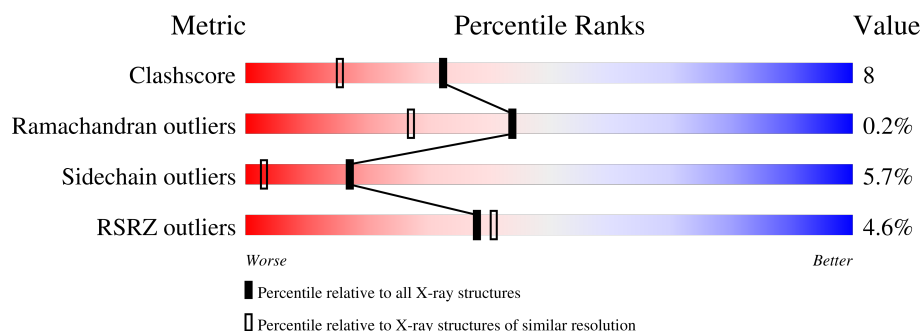
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (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 $\leq 5\%$. 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	439	<div> <div>5%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3837 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 3-phytase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3374	2140	573	646	15			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

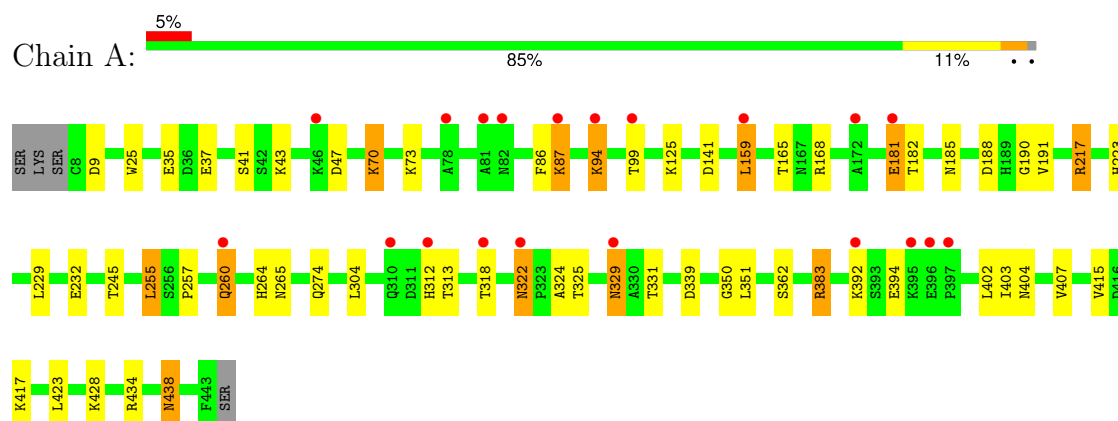
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	397	Total	O	0	0
			397	397		

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: 3-phytase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	39.71Å 99.48Å 100.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.65 30.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	93.5 (30.00-1.65) 90.9 (30.00-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.65 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.175 , 0.231 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.650	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.033 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3837	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: NAG, PO4

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	0.72	1/3455 (0.0%)	0.84	2/4687 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	THR	C-N	8.36	1.53	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	9	ASP	CB-CG-OD2	5.69	123.42	118.30

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	3374	0	3275	53	0
2	A	56	0	52	2	0
3	A	10	0	0	0	0
4	A	397	0	0	20	0
All	All	3837	0	3327	53	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 8.

All (53) 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:260:GLN:HG3	4:A:667:HOH:O	1.69	0.90
1:A:168:ARG:HD2	4:A:712:HOH:O	1.72	0.90
1:A:217:ARG:HH11	1:A:217:ARG:HG2	1.37	0.89
1:A:73:LYS:HE2	4:A:833:HOH:O	1.78	0.81
1:A:232:GLU:HG2	4:A:885:HOH:O	1.84	0.76
1:A:438:ASN:HD22	1:A:438:ASN:H	1.38	0.71
1:A:329:ASN:HD22	1:A:329:ASN:H	1.38	0.69
1:A:402:LEU:CD1	1:A:407:VAL:HG22	2.23	0.68
1:A:181:GLU:HG2	4:A:887:HOH:O	1.97	0.64
1:A:322:ASN:ND2	1:A:325:THR:H	1.96	0.62
1:A:25:TRP:HH2	1:A:255:LEU:HD21	1.64	0.62
1:A:191:VAL:HG22	4:A:567:HOH:O	2.02	0.60
1:A:217:ARG:HD2	1:A:229:LEU:O	2.01	0.60
1:A:402:LEU:HD11	1:A:407:VAL:HG22	1.84	0.59
1:A:159:LEU:HD22	4:A:888:HOH:O	2.03	0.58
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.13	0.58
1:A:87:LYS:HG2	1:A:223:HIS:HA	1.86	0.58
1:A:264:HIS:HD2	4:A:743:HOH:O	1.88	0.56
1:A:274:GLN:HG3	4:A:897:HOH:O	2.06	0.55
1:A:274:GLN:CD	4:A:897:HOH:O	2.46	0.54
1:A:322:ASN:HD21	1:A:324:ALA:HB3	1.73	0.53
1:A:383:ARG:H	1:A:404:ASN:ND2	2.06	0.53
1:A:260:GLN:NE2	4:A:606:HOH:O	1.98	0.53
1:A:304:LEU:HB3	1:A:423:LEU:HD11	1.91	0.53
1:A:329:ASN:HD22	1:A:329:ASN:N	2.03	0.53
1:A:383:ARG:H	1:A:404:ASN:HD21	1.58	0.52
1:A:428:LYS:HA	1:A:434:ARG:NH2	2.26	0.51
1:A:41:SER:OG	1:A:43:LYS:HG3	2.10	0.50
1:A:245:THR:CG2	1:A:255:LEU:HD23	2.41	0.50
1:A:312:HIS:HB3	4:A:729:HOH:O	2.12	0.49
1:A:257:PRO:O	1:A:260:GLN:NE2	2.46	0.48
1:A:434:ARG:HD2	4:A:636:HOH:O	2.13	0.48
1:A:47:ASP:HB3	1:A:392:LYS:HD3	1.94	0.47
1:A:25:TRP:CH2	1:A:255:LEU:HD21	2.48	0.47
1:A:313:THR:O	2:A:503:NAG:H61	2.15	0.46
1:A:185:ASN:O	1:A:188:ASP:O	2.33	0.46
1:A:394:GLU:HB2	4:A:831:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASP:HB3	1:A:392:LYS:HB2	1.97	0.45
1:A:70:LYS:HB2	1:A:70:LYS:HE3	1.82	0.45
1:A:274:GLN:CG	4:A:897:HOH:O	2.65	0.44
1:A:217:ARG:HG2	1:A:217:ARG:NH1	2.18	0.44
1:A:125:LYS:HE2	4:A:790:HOH:O	2.16	0.44
1:A:182:THR:HA	4:A:870:HOH:O	2.16	0.43
1:A:322:ASN:ND2	1:A:325:THR:OG1	2.52	0.43
1:A:350:GLY:HA3	2:A:505:NAG:H82	2.02	0.42
1:A:265:ASN:ND2	4:A:861:HOH:O	2.52	0.41
1:A:351:LEU:HD13	1:A:403:ILE:HD11	2.02	0.41
1:A:402:LEU:HD12	1:A:407:VAL:HG22	2.00	0.41
1:A:87:LYS:HE2	4:A:614:HOH:O	2.20	0.41
1:A:245:THR:HG21	1:A:255:LEU:HD23	2.02	0.41
1:A:86:PHE:CD1	1:A:94:LYS:HG3	2.55	0.41
1:A:94:LYS:HD2	4:A:645:HOH:O	2.20	0.41
1:A:87:LYS:HG3	1:A:223:HIS:HD2	1.87	0.40

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	433/439 (99%)	424 (98%)	8 (2%)	1 (0%)	44 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	GLY

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	366/370 (99%)	345 (94%)	21 (6%)	17 3

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	37	GLU
1	A	70	LYS
1	A	87	LYS
1	A	94	LYS
1	A	99	THR
1	A	141	ASP
1	A	159	LEU
1	A	181	GLU
1	A	217	ARG
1	A	255	LEU
1	A	260	GLN
1	A	318	THR
1	A	322	ASN
1	A	329	ASN
1	A	331	THR
1	A	362	SER
1	A	383	ARG
1	A	415	VAL
1	A	417	LYS
1	A	438	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	HIS
1	A	265	ASN
1	A	322	ASN
1	A	329	ASN

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Mol	Chain	Res	Type
1	A	404	ASN
1	A	438	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	NAG	A	504	1	14,14,15	0.55	0	17,19,21	1.06	2 (11%)
2	NAG	A	503	1	14,14,15	0.78	1 (7%)	17,19,21	2.08	5 (29%)
3	PO4	A	501	-	4,4,4	1.45	1 (25%)	6,6,6	1.23	1 (16%)
2	NAG	A	505	1	14,14,15	0.75	0	17,19,21	1.00	1 (5%)
2	NAG	A	506	1	14,14,15	0.52	0	17,19,21	0.90	0
3	PO4	A	502	-	4,4,4	0.33	0	6,6,6	0.93	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
2	NAG	A	504	1	-	0/6/23/26	0/1/1/1
2	NAG	A	503	1	-	2/6/23/26	0/1/1/1
2	NAG	A	505	1	-	0/6/23/26	0/1/1/1
2	NAG	A	506	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PO4	P-O2	-2.10	1.48	1.54
2	A	503	NAG	C1-C2	2.06	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	NAG	C1-O5-C5	4.69	118.47	112.19
2	A	503	NAG	C6-C5-C4	-3.56	104.28	113.02
2	A	503	NAG	O5-C1-C2	-3.56	105.79	111.29
2	A	505	NAG	C1-O5-C5	2.92	116.11	112.19
2	A	503	NAG	C2-N2-C7	-2.47	119.59	122.90
3	A	501	PO4	O4-P-O2	2.24	114.88	107.91
2	A	504	NAG	C1-O5-C5	2.15	115.07	112.19
2	A	503	NAG	O3-C3-C4	-2.04	105.58	110.38
2	A	504	NAG	C2-N2-C7	-2.01	120.20	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	NAG	C4-C5-C6-O6
2	A	503	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	NAG	1	0
2	A	505	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	435/439 (99%)	0.37	20 (4%) 38 41	13, 23, 36, 44	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	HIS	4.5
1	A	181	GLU	3.7
1	A	159	LEU	3.1
1	A	99	THR	3.0
1	A	322	ASN	2.9
1	A	78	ALA	2.8
1	A	46	LYS	2.7
1	A	395	LYS	2.5
1	A	94	LYS	2.4
1	A	81	ALA	2.4
1	A	87	LYS	2.4
1	A	172	ALA	2.3
1	A	260	GLN	2.3
1	A	397	PRO	2.2
1	A	392	LYS	2.2
1	A	318	THR	2.1
1	A	329	ASN	2.1
1	A	310	GLN	2.0
1	A	82	ASN	2.0
1	A	396	GLU	2.0

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(\AA^2)	Q<0.9
2	NAG	A	504	14/15	0.82	0.12	30,34,37,39	0
2	NAG	A	506	14/15	0.83	0.10	40,43,49,51	0
2	NAG	A	503	14/15	0.87	0.10	24,28,32,33	0
2	NAG	A	505	14/15	0.92	0.08	21,25,32,34	0
3	PO4	A	502	5/5	0.97	0.06	17,18,20,21	0
3	PO4	A	501	5/5	0.98	0.05	17,18,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.