



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:59 AM UTC

PDB ID : 1FX6 / pdb_00001fx6
Title : AQUIFEX AEOLICUS KDO8P SYNTHASE
Authors : Duewel, H.S.; Radaev, S.; Wang, J.; Woodard, R.W.; Gatti, D.L.
Deposited on : 2000-09-25
Resolution : 2.06 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

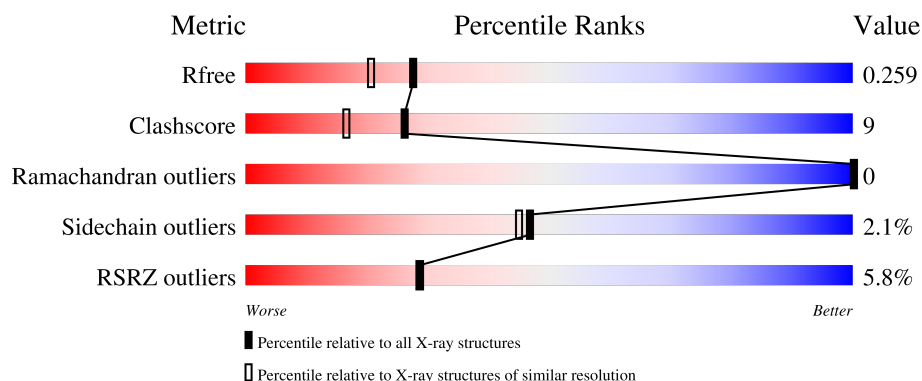
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	267	
1	B	267	

2 Entry composition [i](#)

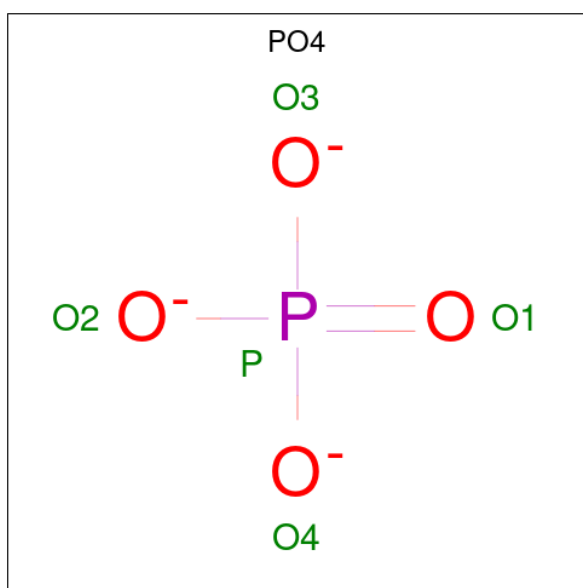
There are 3 unique types of molecules in this entry. The entry contains 4227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-DEHYDRO-3-DEOXYPHOSPHOONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1990	1286	331	367	6			
1	B	249	Total	C	N	O	S	0	0	0
			1973	1276	329	363	5			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total 146	O 146	0	0
3	B	108	Total 108	O 108	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.59Å 84.59Å 159.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.05 – 2.06 43.05 – 2.06	Depositor EDS
% Data completeness (in resolution range)	81.7 (43.05-2.06) 81.9 (43.05-2.06)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.06Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.216 , 0.259 0.216 , 0.259	Depositor DCC
R_{free} test set	3396 reflections (8.81%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4227	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	0/2029	0.88	4/2736 (0.1%)
1	B	0.39	0/2012	0.87	1/2714 (0.0%)
All	All	0.40	0/4041	0.88	5/5450 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1179	VAL	N-CA-C	6.46	117.22	108.17
1	A	1149	ILE	N-CA-C	6.00	116.51	108.11
1	A	1115	ALA	N-CA-C	5.90	117.71	111.28
1	B	2179	VAL	N-CA-C	5.58	115.92	108.11
1	A	1258	SER	N-CA-C	5.52	118.82	111.75

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	1990	0	2026	28	0
1	B	1973	0	2011	51	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	146	0	0	1	0
3	B	108	0	0	5	0
All	All	4227	0	4037	75	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 9.

All (75) 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:2020:LEU:HD21	1:B:2069:LYS:HG3	1.55	0.88
1:A:1161:ASN:HD21	1:B:2132:TRP:HE1	1.23	0.86
1:B:2208:ILE:HD11	1:B:2219:VAL:HG11	1.59	0.83
1:A:1132:TRP:HE1	1:B:2161:ASN:HD21	1.23	0.82
1:B:2011:CYS:H	1:B:2237:GLN:NE2	1.76	0.82
1:B:2263:THR:O	1:B:2264:ILE:HG22	1.88	0.73
1:A:1228:GLU:HG2	3:A:3267:HOH:O	1.90	0.71
1:A:1041:LYS:HD3	1:A:1041:LYS:C	2.21	0.65
1:B:2041:LYS:HD3	1:B:2041:LYS:C	2.25	0.62
1:A:1174:LYS:HG3	1:A:1264:ILE:HG21	1.83	0.60
1:A:1100:ILE:HG13	1:A:1111:LEU:HD23	1.85	0.59
1:B:2025:GLU:HG2	1:B:2240:LEU:HD22	1.83	0.58
1:B:2208:ILE:CD1	1:B:2219:VAL:HG11	2.30	0.58
1:B:2011:CYS:H	1:B:2237:GLN:HE22	1.52	0.57
1:A:1201:ARG:HG3	1:A:1204:ILE:HD12	1.87	0.57
1:B:2185:HIS:HE1	1:B:2222:GLU:CD	2.13	0.56
1:B:2205:PHE:O	1:B:2208:ILE:HG22	2.06	0.54
1:B:2093:GLU:HG3	3:B:3123:HOH:O	2.07	0.54
1:B:2147:LYS:HB3	1:B:2147:LYS:NZ	2.23	0.54
1:A:1233:ASP:O	1:A:1237:GLN:HG3	2.07	0.54
1:A:1205:PHE:O	1:A:1208:ILE:HG22	2.09	0.53
1:B:2234:ALA:HB3	3:B:3219:HOH:O	2.09	0.53
1:A:1048:ASN:H	1:A:1048:ASN:HD22	1.58	0.52
1:B:2068:ARG:O	1:B:2072:GLU:HG3	2.09	0.52
1:B:2029:LEU:HD11	1:B:2244:GLU:HB2	1.91	0.51
1:B:2041:LYS:HD3	1:B:2042:SER:N	2.26	0.51
1:B:2013:ILE:HG23	1:B:2019:LEU:HD11	1.93	0.50
1:B:2201:ARG:N	3:B:3188:HOH:O	2.43	0.50
1:B:2081:ASP:HB3	1:B:2099:GLN:HB3	1.93	0.50
1:A:1060:LEU:C	1:A:1060:LEU:HD13	2.37	0.50
1:B:2031:GLU:O	1:B:2034:LYS:HE2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:LYS:HG3	1:A:1264:ILE:HD13	1.93	0.49
1:B:2205:PHE:HB3	1:B:2206:PRO:HD3	1.93	0.49
1:B:2172:ILE:O	1:B:2175:GLN:HG3	2.13	0.48
1:B:2029:LEU:HD12	1:B:2033:PHE:HE1	1.78	0.48
1:B:2005:LEU:HD12	1:B:2037:GLU:HB3	1.94	0.48
1:B:2182:ASP:HA	1:B:2220:PHE:HB3	1.94	0.48
1:A:1041:LYS:HD3	1:A:1042:SER:N	2.28	0.47
1:A:1097:ILE:HG12	1:A:1120:ALA:HB3	1.96	0.47
1:B:2044:PHE:CZ	1:B:2060:LEU:HD13	2.49	0.47
1:B:2055:PHE:CZ	1:B:2057:GLY:HA2	2.49	0.47
1:A:1154:ARG:O	1:A:1154:ARG:HD3	2.15	0.47
1:B:2078:ILE:HG22	1:B:2079:THR:N	2.27	0.47
1:B:2040:PHE:HB3	1:B:2078:ILE:HD13	1.97	0.46
1:B:2011:CYS:HB3	3:B:3147:HOH:O	2.16	0.46
1:B:2258:SER:HA	1:B:2261:TYR:CE2	2.51	0.45
1:B:2025:GLU:O	1:B:2029:LEU:HD22	2.16	0.45
1:A:1187:VAL:HG12	1:A:1207:LEU:HD12	1.99	0.45
1:B:2233:ASP:HB3	1:B:2236:THR:OG1	2.16	0.45
1:B:2048:ASN:H	1:B:2048:ASN:HD22	1.64	0.45
1:B:2238:LEU:HD21	1:B:2246:ILE:HD12	1.97	0.45
1:A:1044:PHE:CZ	1:A:1060:LEU:HD23	2.51	0.45
1:B:2212:VAL:HG11	1:B:2250:ILE:HB	1.98	0.45
1:B:2060:LEU:O	1:B:2064:VAL:HG23	2.16	0.45
1:B:2099:GLN:NE2	1:B:2220:PHE:HE2	2.15	0.45
1:A:1030:SER:HA	1:A:1038:PHE:CE1	2.52	0.44
1:A:1205:PHE:HB3	1:A:1206:PRO:CD	2.48	0.44
1:B:2258:SER:HA	1:B:2261:TYR:CD2	2.53	0.43
1:B:2187:VAL:O	1:B:2187:VAL:HG23	2.19	0.43
1:A:1212:VAL:HG11	1:A:1250:ILE:HB	2.01	0.43
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.15	0.42
1:B:2099:GLN:HE22	1:B:2220:PHE:HE2	1.67	0.42
1:B:2078:ILE:CG2	1:B:2079:THR:N	2.82	0.42
1:A:1106:ARG:HD2	1:B:2048:ASN:O	2.20	0.42
1:A:1130:ALA:HB3	1:A:1133:ASP:OD2	2.20	0.42
1:A:1045:ASP:OD2	1:A:1047:ALA:HB2	2.20	0.41
1:A:1140:LYS:HG2	1:B:2052:ILE:HB	2.00	0.41
1:A:1005:LEU:HD12	1:A:1037:GLU:HB3	2.03	0.41
1:B:2016:GLU:O	1:B:2020:LEU:HG	2.21	0.41
1:B:2232:SER:O	1:B:2233:ASP:C	2.64	0.40
1:B:2027:LYS:O	1:B:2030:SER:HB3	2.21	0.40
1:B:2031:GLU:OE1	1:B:2034:LYS:NZ	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2106:ARG:HB2	3:B:3019:HOH:O	2.21	0.40
1:A:1055:PHE:CE1	1:A:1231:LEU:HD13	2.56	0.40
1:A:1089:GLU:HB3	1:A:1090:PRO:CD	2.52	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	247/267 (92%)	243 (98%)	4 (2%)	0	100	100
1	B	245/267 (92%)	233 (95%)	12 (5%)	0	100	100
All	All	492/534 (92%)	476 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	213/224 (95%)	208 (98%)	5 (2%)	44	41
1	B	211/224 (94%)	207 (98%)	4 (2%)	50	49
All	All	424/448 (95%)	415 (98%)	9 (2%)	47	45

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1048	ASN
1	A	1076	LEU
1	A	1106	ARG
1	A	1112	LEU
1	A	1124	LYS
1	B	2029	LEU
1	B	2048	ASN
1	B	2147	LYS
1	B	2240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1048	ASN
1	A	1058	HIS
1	A	1161	ASN
1	A	1162	ASN
1	A	1175	GLN
1	B	2048	ASN
1	B	2099	GLN
1	B	2122	ASN
1	B	2136	ASN
1	B	2161	ASN
1	B	2162	ASN
1	B	2185	HIS
1	B	2237	GLN

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 [i](#)

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	PO4	B	2268	-	4,4,4	1.67	0	6,6,6	0.47	0
2	PO4	A	1268	-	4,4,4	1.69	0	6,6,6	0.47	0

There are no bond length outliers.

There are no bond angle outliers.

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, 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	251/267 (94%)	0.16	11 (4%) 39 39	9, 23, 44, 54	0
1	B	249/267 (93%)	0.55	18 (7%) 21 21	14, 28, 50, 69	0
All	All	500/534 (93%)	0.36	29 (5%) 29 28	9, 25, 46, 69	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2234	ALA	6.5
1	B	2235	SER	5.8
1	B	2264	ILE	5.2
1	B	2232	SER	4.4
1	B	2236	THR	4.3
1	A	1264	ILE	4.1
1	A	1200	MET	4.1
1	B	2233	ASP	4.0
1	B	2231	LEU	3.7
1	B	2230	ALA	3.4
1	B	2060	LEU	3.2
1	A	1235	SER	3.0
1	B	2176	TRP	2.6
1	A	1220	PHE	2.6
1	A	1201	ARG	2.6
1	B	2187	VAL	2.5
1	B	2055	PHE	2.5
1	B	2147	LYS	2.5
1	B	2035	GLU	2.4
1	A	1050	SER	2.3
1	A	1228	GLU	2.2
1	A	1072	GLU	2.2
1	B	2227	PRO	2.2
1	B	2228	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1187	VAL	2.1
1	B	2034	LYS	2.1
1	A	1233	ASP	2.1
1	A	1231	LEU	2.0
1	B	2094	VAL	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PO4	B	2268	5/5	0.95	0.13	36,38,40,40	0
2	PO4	A	1268	5/5	0.97	0.10	33,34,35,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.