



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 06:16 PM EST

PDB ID : 3QK6
Title : Crystal structure of Escherichia coli PhnD
Authors : Alicea, I.; Schreiter, E.R.
Deposited on : 2011-01-31
Resolution : 2.40 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	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

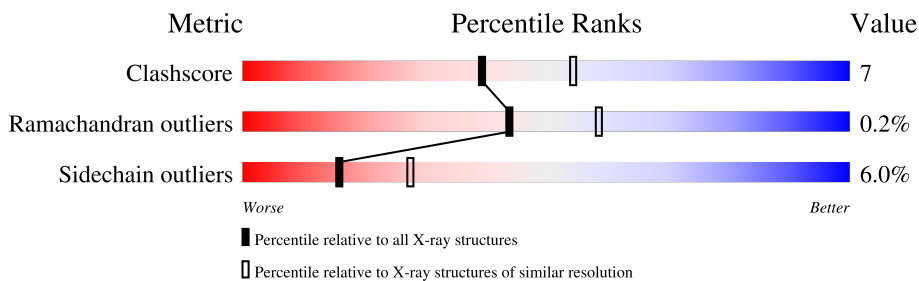
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)

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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	321	
1	B	321	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNL	A	313	-	-	X	-
2	UNL	B	313	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4828 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 PhnD, subunit of alkylphosphonate ABC transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	Se	0	0	0
			2380	1512	407	455	6			
1	B	308	Total	C	N	O	Se	0	0	0
			2409	1530	413	460	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MSE	-	expression tag	UNP Q1R3F7
A	-7	HIS	-	expression tag	UNP Q1R3F7
A	-6	HIS	-	expression tag	UNP Q1R3F7
A	-5	HIS	-	expression tag	UNP Q1R3F7
A	-4	HIS	-	expression tag	UNP Q1R3F7
A	-3	HIS	-	expression tag	UNP Q1R3F7
A	-2	HIS	-	expression tag	UNP Q1R3F7
A	-1	GLY	-	expression tag	UNP Q1R3F7
A	0	SER	-	expression tag	UNP Q1R3F7
B	-8	MSE	-	expression tag	UNP Q1R3F7
B	-7	HIS	-	expression tag	UNP Q1R3F7
B	-6	HIS	-	expression tag	UNP Q1R3F7
B	-5	HIS	-	expression tag	UNP Q1R3F7
B	-4	HIS	-	expression tag	UNP Q1R3F7
B	-3	HIS	-	expression tag	UNP Q1R3F7
B	-2	HIS	-	expression tag	UNP Q1R3F7
B	-1	GLY	-	expression tag	UNP Q1R3F7
B	0	SER	-	expression tag	UNP Q1R3F7

- Molecule 2 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	X	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	X	0	0
			5	5		

- Molecule 3 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	13	Total	O	0	0
			13	13		
3	B	16	Total	O	0	0
			16	16		

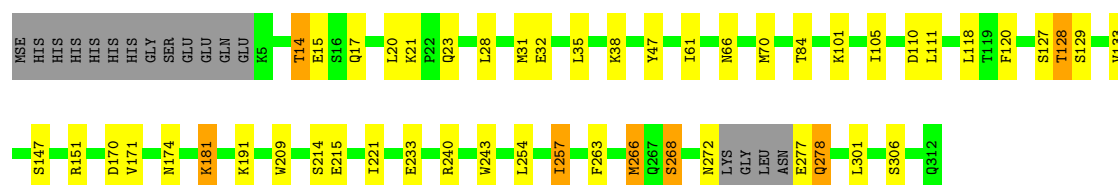
3 Residue-property plots

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.

Note EDS failed to run properly.

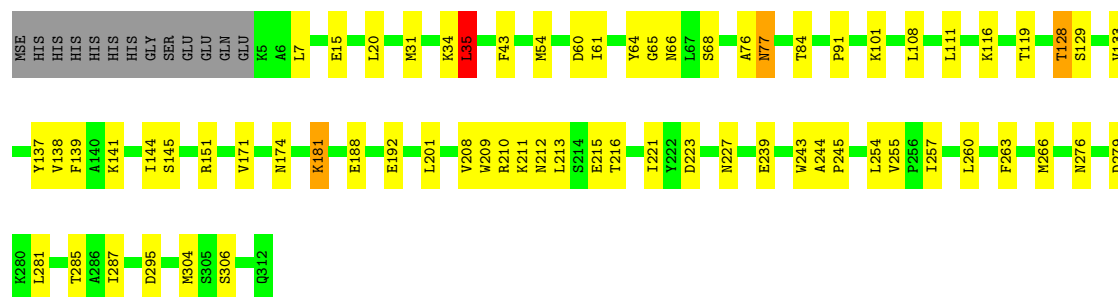
- Molecule 1: PhnD, subunit of alkylphosphonate ABC transporter

Chain A: 



- Molecule 1: PhnD, subunit of alkylphosphonate ABC transporter

Chain B: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.74Å 82.98Å 66.14Å 90.00° 103.20° 90.00°	Depositor
Resolution (Å)	43.00 – 2.40	Depositor
% Data completeness (in resolution range)	93.9 (43.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.206 , 0.267	Depositor
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.628	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4828	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: UNL

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	0.82	0/2420	0.82	0/3266
1	B	0.82	2/2450 (0.1%)	0.80	1/3307 (0.0%)
All	All	0.82	2/4870 (0.0%)	0.81	1/6573 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	PHE	CE2-CZ	5.71	1.48	1.37
1	B	43	PHE	CG-CD1	5.39	1.46	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	LEU	CA-CB-CG	5.14	127.13	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	2380	0	2384	31	0
1	B	2409	0	2418	33	0
2	A	5	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	5	0
3	A	13	0	0	0	0
3	B	16	0	0	0	0
All	All	4828	0	4802	63	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 7.

All (63) 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:128:THR:H	2:B:313:UNL:X3	1.92	0.82
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.51	0.75
1:A:128:THR:H	2:A:313:UNL:X2	2.03	0.70
1:B:128:THR:OG1	2:B:313:UNL:X3	2.44	0.65
1:B:139:PHE:HB3	1:B:144:ILE:O	1.95	0.65
1:A:268:SER:O	1:A:272:ASN:HB2	1.96	0.65
1:A:47:TYR:OH	2:A:313:UNL:X3	2.45	0.64
1:A:101:LYS:HE3	1:A:191:LYS:O	1.98	0.62
1:B:263:PHE:O	1:B:266:MSE:HB3	2.01	0.60
1:A:15:GLU:OE1	1:A:181:LYS:HG2	2.02	0.59
1:B:108:LEU:HD11	1:B:138:VAL:HG13	1.85	0.59
1:A:240:ARG:O	1:A:240:ARG:HG2	2.03	0.58
1:A:61:ILE:HD11	1:A:221:ILE:CD1	2.33	0.58
1:A:32:GLU:OE2	1:A:38:LYS:HA	2.04	0.58
1:A:17:GLN:O	1:A:21:LYS:HG3	2.06	0.56
1:B:129:SER:H	2:B:313:UNL:X5	2.18	0.56
1:B:64:TYR:HD1	1:B:68:SER:HG	1.53	0.56
1:B:31:MSE:HG2	1:B:35:LEU:HD22	1.88	0.55
1:B:60:ASP:OD1	1:B:210:ARG:NH2	2.38	0.55
1:B:111:LEU:HD11	1:B:171:VAL:HG11	1.89	0.55
1:B:119:THR:HG22	1:B:151:ARG:HB3	1.89	0.54
1:A:61:ILE:HD11	1:A:221:ILE:HD13	1.91	0.53
1:A:151:ARG:HG2	1:A:151:ARG:NH1	2.22	0.53
1:B:66:ASN:HB3	1:B:257:ILE:HG12	1.91	0.52
1:B:61:ILE:HD11	1:B:221:ILE:CD1	2.41	0.50
1:B:15:GLU:OE1	1:B:181:LYS:HG2	2.11	0.50
1:B:101:LYS:HD3	1:B:192:GLU:HA	1.94	0.50
1:B:137:TYR:HA	1:B:141:LYS:HG3	1.93	0.49
1:A:128:THR:O	1:A:133:VAL:HG23	2.13	0.48
1:B:129:SER:OG	2:B:313:UNL:X5	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLU:OE2	1:A:38:LYS:HD2	2.13	0.48
1:A:66:ASN:HB3	1:A:257:ILE:HG13	1.95	0.48
1:A:263:PHE:O	1:A:266:MSE:HB3	2.14	0.47
1:B:60:ASP:OD1	1:B:210:ARG:NE	2.46	0.47
1:B:84:THR:HG21	1:B:243:TRP:CZ2	2.49	0.47
1:B:281:LEU:O	1:B:285:THR:HG23	2.15	0.47
1:A:129:SER:OG	2:A:313:UNL:X4	2.63	0.47
1:A:120:PHE:HD1	1:A:171:VAL:HG13	1.79	0.46
1:A:14:THR:HG22	1:A:20:LEU:HD21	1.98	0.46
1:A:23:GLN:HA	1:A:240:ARG:CD	2.46	0.46
1:B:76:ALA:O	1:B:77:ASN:CB	2.61	0.45
1:B:133:VAL:HG22	1:B:260:LEU:HD21	1.97	0.45
1:A:105:ILE:HG23	1:A:110:ASP:HB2	1.99	0.45
1:B:266:MSE:HE2	1:B:287:ILE:HG22	1.99	0.45
1:B:276:ASN:HB2	1:B:279:ASP:H	1.81	0.45
1:A:278:GLN:H	1:A:278:GLN:HG2	1.69	0.44
1:A:28:LEU:O	1:A:32:GLU:HG3	2.19	0.43
1:B:91:PRO:HG2	1:B:201:LEU:HD21	2.00	0.42
1:B:15:GLU:O	1:B:20:LEU:HD11	2.19	0.42
1:B:65:GLY:HA3	2:B:313:UNL:X3	2.49	0.42
1:A:70:MSE:HA	1:A:254:LEU:HD13	2.00	0.42
1:A:84:THR:HG21	1:A:243:TRP:CZ2	2.55	0.42
1:A:127:SER:OG	2:A:313:UNL:X3	2.67	0.42
1:B:54:MSE:HE1	1:B:208:VAL:HG12	2.01	0.42
1:A:111:LEU:HD11	1:A:171:VAL:HG11	2.02	0.42
1:A:118:LEU:HD22	1:A:170:ASP:HB3	2.02	0.42
1:B:211:LYS:C	1:B:213:LEU:H	2.24	0.41
1:A:301:LEU:HD22	1:B:304:MSE:HE1	2.01	0.41
1:A:31:MSE:HG2	1:A:35:LEU:HD22	2.01	0.41
1:B:254:LEU:O	1:B:255:VAL:C	2.59	0.41
1:B:244:ALA:HB1	1:B:245:PRO:HD2	2.02	0.41
1:B:223:ASP:OD2	1:B:227:ASN:ND2	2.54	0.40
1:A:23:GLN:HA	1:A:240:ARG:HD3	2.02	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	300/321 (94%)	290 (97%)	10 (3%)	0	100	100
1	B	306/321 (95%)	293 (96%)	12 (4%)	1 (0%)	37	51
All	All	606/642 (94%)	583 (96%)	22 (4%)	1 (0%)	44	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	212	ASN

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	258/266 (97%)	243 (94%)	15 (6%)	17	29
1	B	261/266 (98%)	245 (94%)	16 (6%)	15	27
All	All	519/532 (98%)	488 (94%)	31 (6%)	16	27

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	128	THR
1	A	147	SER
1	A	174	ASN
1	A	181	LYS

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Mol	Chain	Res	Type
1	A	209	TRP
1	A	214	SER
1	A	215	GLU
1	A	233	GLU
1	A	257	ILE
1	A	266	MSE
1	A	268	SER
1	A	277	GLU
1	A	278	GLN
1	A	306	SER
1	B	7	LEU
1	B	34	LYS
1	B	35	LEU
1	B	77	ASN
1	B	116	LYS
1	B	128	THR
1	B	145	SER
1	B	174	ASN
1	B	181	LYS
1	B	188	GLU
1	B	209	TRP
1	B	215	GLU
1	B	216	THR
1	B	239	GLU
1	B	295	ASP
1	B	306	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	57	ASN
1	B	299	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are unknown - leaving 0 for Mogul analysis.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.