Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 04:54 PM EDT

PDB ID	:	2QIK
Title	:	Crystal structure of YkqA from Bacillus subtilis. Northeast Structural Genomics Target SR631
Authors	:	Benach, J.; Chen, Y.; Forouhar, F.; Seetharaman, J.; Baran, M.C.; Cunningham, K.; Ma, L.-C.; Owens, L.; Chen, C.X.; Rong, X.; Janjua, H.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2007-07-05
Resolution	:	1.35 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 (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 (i)) were used in the production of this report:

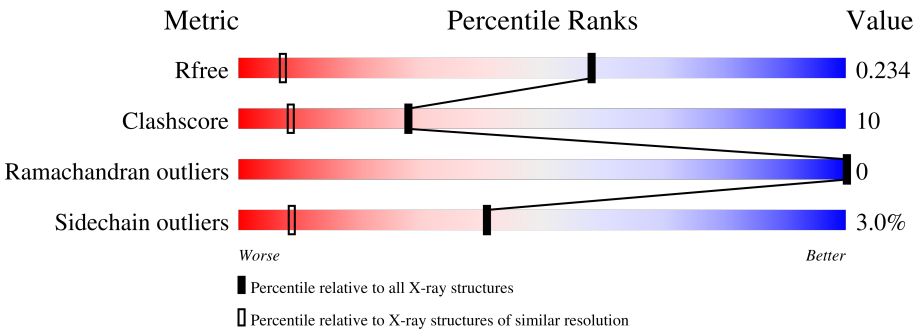
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)

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%

Mol	Chain	Length	Quality of chain
1	A	285	

Validation Pipeline (wwPDB-VP) : 2.37.1

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2686 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.

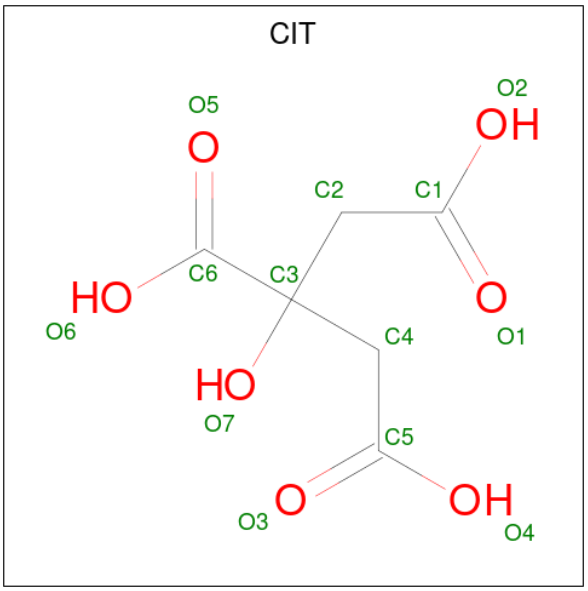
- Molecule 1 is a protein called UPF0131 protein ykqA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	269	2227	1435	372	410	4	6	0	10	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P39759
A	100	MSE	MET	MODIFIED RESIDUE	UNP P39759
A	121	MSE	MET	MODIFIED RESIDUE	UNP P39759
A	138	MSE	MET	MODIFIED RESIDUE	UNP P39759
A	180	MSE	MET	MODIFIED RESIDUE	UNP P39759
A	272	MSE	MET	MODIFIED RESIDUE	UNP P39759
A	279	LEU	-	CLONING ARTIFACT	UNP P39759
A	280	GLU	-	CLONING ARTIFACT	UNP P39759
A	281	HIS	-	CLONING ARTIFACT	UNP P39759
A	282	HIS	-	CLONING ARTIFACT	UNP P39759
A	283	HIS	-	CLONING ARTIFACT	UNP P39759
A	284	HIS	-	CLONING ARTIFACT	UNP P39759
A	285	HIS	-	CLONING ARTIFACT	UNP P39759
A	286	HIS	-	CLONING ARTIFACT	UNP P39759

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	6	7	0	0

- Molecule 3 is water.

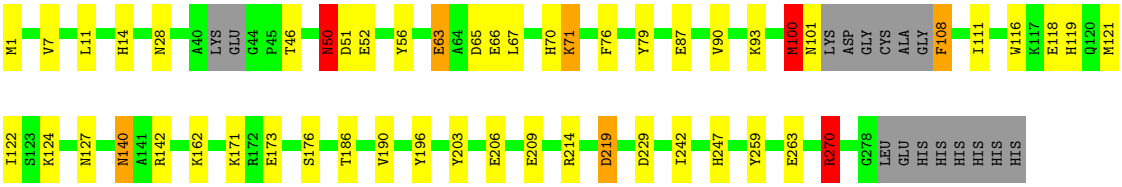
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	446	446	446	0	0

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. 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. 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: UPF0131 protein ykqA

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	38.58Å 62.13Å 55.53Å 90.00° 101.69° 90.00°	Depositor
Resolution (Å)	19.35 – 1.35 19.35 – 1.35	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.35-1.35) 97.8 (19.35-1.35)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.08 (at 1.35Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.131 , 0.176 0.213 , 0.234	Depositor DCC
R_{free} test set	2832 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	10.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 56.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2686	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.18% 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 (i)

5.1 Standard geometry (i)

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

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	1.25	14/2304 (0.6%)	1.10	8/3094 (0.3%)

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
1	A	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	ASN	CG-OD1	-10.53	1.00	1.24
1	A	270	ARG	CG-CD	8.61	1.73	1.51
1	A	56	TYR	CE1-CZ	-7.57	1.28	1.38
1	A	63	GLU	CG-CD	-7.39	1.40	1.51
1	A	263	GLU	CD-OE1	7.29	1.33	1.25
1	A	87	GLU	CD-OE2	6.81	1.33	1.25
1	A	71	LYS	CD-CE	-6.39	1.35	1.51
1	A	63	GLU	CD-OE2	6.25	1.32	1.25
1	A	214	ARG	CZ-NH2	-6.09	1.25	1.33
1	A	214	ARG	NE-CZ	6.04	1.40	1.33
1	A	116	TRP	CE3-CZ3	5.85	1.48	1.38
1	A	206	GLU	CG-CD	-5.70	1.43	1.51
1	A	87	GLU	CD-OE1	-5.48	1.19	1.25
1	A	66	GLU	CD-OE1	-5.28	1.19	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	63	GLU	OE1-CD-OE2	8.15	133.09	123.30
1	A	142	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	A	51	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	65	ASP	CB-CG-OD2	6.87	124.48	118.30
1	A	100	MSE	CA-CB-CG	6.34	124.08	113.30
1	A	229	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	219	ASP	CB-CG-OD1	5.14	122.93	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	ASN	Sidechain
1	A	90	VAL	Mainchain

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	2227	0	2213	44	0
2	A	13	0	5	0	0
3	A	446	0	0	14	0
All	All	2686	0	2218	44	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 10.

All (44) 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:7[B]:VAL:HG11	1:A:11:LEU:HB2	1.39	1.02
1:A:7[B]:VAL:CG1	1:A:11:LEU:HB2	1.91	1.01
1:A:124:LYS:NZ	3:A:473:HOH:O	2.00	0.93
1:A:7[B]:VAL:HG11	1:A:11:LEU:CB	2.04	0.86
1:A:28:ASN:HD21	1:A:93[A]:LYS:HE3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PHE:HE2	3:A:747:HOH:O	1.76	0.67
1:A:190:VAL:HG21	1:A:259:TYR:CD2	2.28	0.67
1:A:63:GLU:OE1	3:A:548:HOH:O	2.12	0.66
1:A:79:TYR:OH	1:A:100:MSE:HE2	1.96	0.66
1:A:270:ARG:HH21	1:A:270:ARG:HB3	1.61	0.66
1:A:67:LEU:HD21	1:A:71:LYS:HD2	1.76	0.66
1:A:176[B]:SER:OG	1:A:242:ILE:HG12	1.95	0.66
1:A:186[B]:THR:HG21	3:A:555:HOH:O	1.97	0.64
1:A:70:HIS:HE1	3:A:348:HOH:O	1.80	0.63
1:A:14:HIS:HE1	1:A:219:ASP:OD2	1.82	0.62
1:A:108:PHE:N	1:A:108:PHE:CD2	2.67	0.61
1:A:173:GLU:HG3	3:A:500:HOH:O	2.00	0.61
1:A:50:ASN:HD21	1:A:52:GLU:H	1.48	0.61
1:A:50:ASN:ND2	1:A:52:GLU:H	1.99	0.61
1:A:7[B]:VAL:HG13	1:A:11:LEU:HB2	1.78	0.61
1:A:70:HIS:HD2	3:A:384:HOH:O	1.84	0.61
1:A:14:HIS:HD2	3:A:619:HOH:O	1.85	0.60
1:A:67:LEU:CD2	1:A:71:LYS:HD2	2.32	0.59
1:A:63:GLU:CD	3:A:548:HOH:O	2.45	0.55
1:A:127:ASN:ND2	1:A:196:TYR:H	2.06	0.54
1:A:171:LYS:HD2	1:A:171:LYS:C	2.29	0.53
1:A:28:ASN:HD21	1:A:93[B]:LYS:NZ	2.06	0.53
1:A:186[B]:THR:HG23	3:A:554:HOH:O	2.09	0.51
1:A:162[B]:LYS:HE2	3:A:555:HOH:O	2.10	0.50
1:A:186[B]:THR:HG22	3:A:434:HOH:O	2.14	0.47
1:A:28:ASN:HD21	1:A:93[B]:LYS:HZ2	1.62	0.46
1:A:190:VAL:CG2	1:A:259:TYR:CD2	2.98	0.46
1:A:247:HIS:HB2	3:A:557:HOH:O	2.14	0.46
1:A:176[B]:SER:OG	1:A:242:ILE:CG1	2.63	0.45
1:A:209:GLU:HG3	3:A:709:HOH:O	2.15	0.45
1:A:79:TYR:CZ	1:A:100:MSE:HG2	2.52	0.45
1:A:46:THR:CB	1:A:100:MSE:HG3	2.47	0.44
1:A:127:ASN:HD22	1:A:196:TYR:H	1.64	0.44
1:A:140:ASN:H	1:A:140:ASN:HD22	1.64	0.44
1:A:79:TYR:OH	1:A:100:MSE:CE	2.65	0.42
1:A:111[A]:ILE:HD12	1:A:119:HIS:CD2	2.55	0.42
1:A:121:MSE:HE3	1:A:122[A]:ILE:HD11	2.01	0.41
1:A:118:GLU:O	1:A:122[A]:ILE:HD12	2.21	0.41
1:A:122[A]:ILE:HD11	1:A:203:TYR:OH	2.21	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	273/285 (96%)	267 (98%)	6 (2%)	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	240/237 (101%)	233 (97%)	7 (3%)	42 10

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	50	ASN
1	A	100	MSE
1	A	101	ASN
1	A	108	PHE
1	A	140	ASN
1	A	270	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN

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Mol	Chain	Res	Type
1	A	14	HIS
1	A	19	HIS
1	A	28	ASN
1	A	50	ASN
1	A	70	HIS
1	A	74	GLN
1	A	119	HIS
1	A	120	GLN
1	A	127	ASN
1	A	140	ASN
1	A	153	GLN
1	A	246	GLN
1	A	249	GLN
1	A	273	ASN

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)

1 ligand is 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	CIT	A	301	-	12,12,12	2.25	3 (25%)	17,17,17	1.67	3 (17%)

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	CIT	A	301	-	-	0/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CIT	C3-C6	-5.89	1.47	1.53
2	A	301	CIT	O7-C3	3.02	1.49	1.43
2	A	301	CIT	C4-C3	-2.03	1.51	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	CIT	O5-C6-C3	-3.37	115.57	122.09
2	A	301	CIT	O6-C6-C3	3.26	119.39	113.14
2	A	301	CIT	C4-C3-C6	2.73	116.08	110.03

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.