Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2024 – 03:05 AM EST

PDB ID	:	2BDT
Title	:	Crystal Structure of the Putative Gluconate Kinase from Bacillus halodurans, Northeast Structural Genomics Target BhR61
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Deposited on	:	2005-10-20
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:

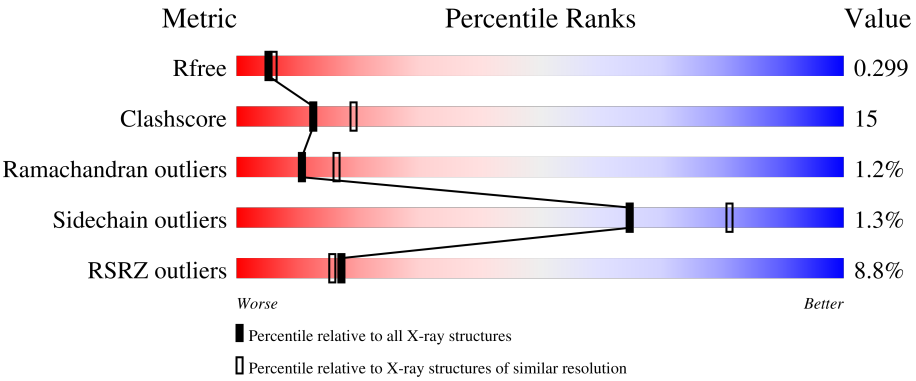
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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))
R_{free}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (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 <=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	189	8%, 62%, 29%, 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1432 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.

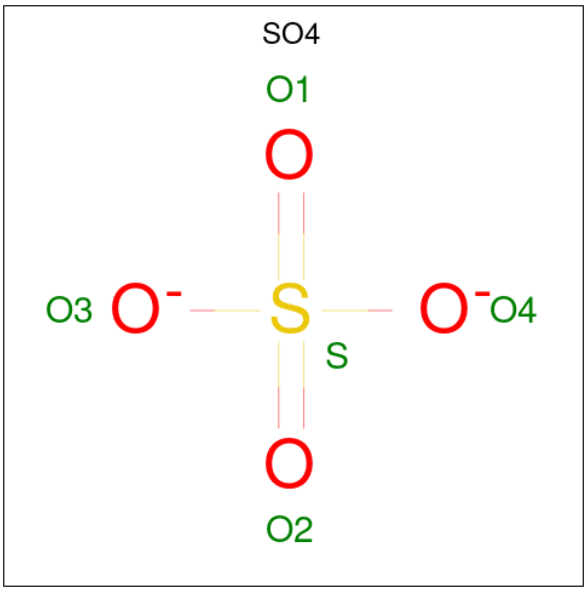
- Molecule 1 is a protein called BH3686.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	172	1391	888	236	262	3	2	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9K6P2
A	40	MSE	MET	modified residue	UNP Q9K6P2
A	128	MSE	MET	modified residue	UNP Q9K6P2
A	177	MSE	-	SEE REMARK 999	UNP Q9K6P2
A	178	ALA	-	cloning artifact	UNP Q9K6P2
A	179	GLY	-	cloning artifact	UNP Q9K6P2
A	180	ASP	-	cloning artifact	UNP Q9K6P2
A	181	PRO	-	cloning artifact	UNP Q9K6P2
A	182	LEU	-	cloning artifact	UNP Q9K6P2
A	183	GLU	-	cloning artifact	UNP Q9K6P2
A	184	HIS	-	expression tag	UNP Q9K6P2
A	185	HIS	-	expression tag	UNP Q9K6P2
A	186	HIS	-	expression tag	UNP Q9K6P2
A	187	HIS	-	expression tag	UNP Q9K6P2
A	188	HIS	-	expression tag	UNP Q9K6P2
A	189	HIS	-	expression tag	UNP Q9K6P2

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

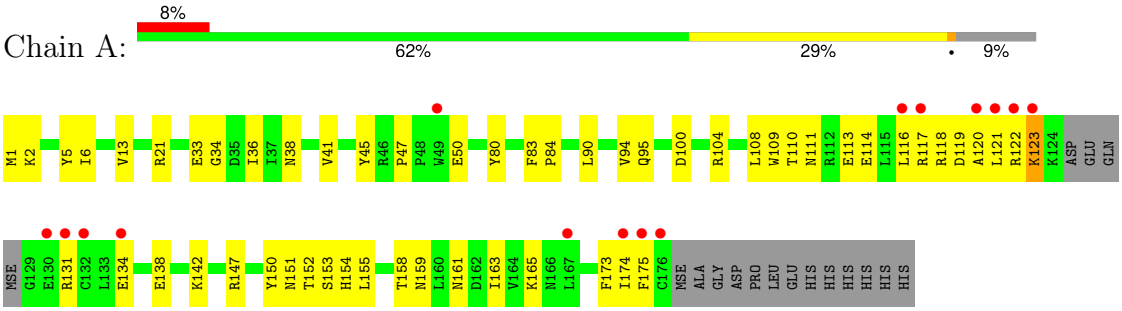
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	36	Total O 36 36	0	0

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 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: BH3686

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	43.67Å 43.67Å 198.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.81 – 2.40 32.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	85.7 (32.81-2.40) 87.0 (32.81-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.18 (at 1.75Å)	Xtriage
Refinement program	CNS 1.1, XTALVIEW	Depositor
R, R_{free}	0.233 , 0.287 0.248 , 0.299	Depositor DCC
R_{free} test set	707 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	1432	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 8.05% 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: SO4

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	0.36	0/1415	0.51	0/1915

There are no bond length outliers.

There are no bond angle outliers.

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	1391	0	1396	42	0
2	A	5	0	0	0	0
3	A	36	0	0	1	0
All	All	1432	0	1396	42	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 15.

All (42) 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:41:VAL:HG13	1:A:45:TYR:HD1	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:O	1:A:116:LEU:HB3	1.87	0.74
1:A:33:GLU:O	1:A:36:ILE:HG22	1.91	0.70
1:A:152:THR:HA	1:A:155:LEU:HD23	1.76	0.68
1:A:21:ARG:HH11	1:A:161:ASN:HD21	1.43	0.64
1:A:111:ASN:HB3	1:A:114:GLU:HG2	1.79	0.64
1:A:47:PRO:HG2	1:A:50:GLU:HG3	1.80	0.62
1:A:116:LEU:HD21	1:A:117:ARG:NH2	2.19	0.57
1:A:173:PHE:C	1:A:175:PHE:H	2.08	0.56
1:A:173:PHE:O	1:A:175:PHE:N	2.38	0.55
1:A:131:ARG:O	1:A:131:ARG:HD2	2.07	0.54
1:A:110:THR:O	1:A:153:SER:HB3	2.08	0.53
1:A:131:ARG:HA	1:A:134:GLU:HG3	1.90	0.53
1:A:34:GLY:HA3	1:A:80:TYR:CD2	2.43	0.53
1:A:158:THR:HG23	1:A:159:ASN:ND2	2.24	0.52
1:A:150:TYR:CE1	1:A:163:ILE:HG23	2.45	0.52
1:A:121:LEU:HD12	1:A:121:LEU:N	2.25	0.51
1:A:109:TRP:O	1:A:151:ASN:HA	2.11	0.50
1:A:5:TYR:CE1	1:A:104:ARG:HD2	2.46	0.49
1:A:150:TYR:HE1	1:A:163:ILE:HG23	1.77	0.49
1:A:120:ALA:C	1:A:121:LEU:HD12	2.34	0.48
1:A:83:PHE:HB3	1:A:84:PRO:HD2	1.95	0.48
1:A:111:ASN:HB3	1:A:114:GLU:CG	2.44	0.48
1:A:116:LEU:HD21	1:A:117:ARG:HH21	1.79	0.47
1:A:6:ILE:HD11	1:A:90:LEU:HD23	1.97	0.47
1:A:38:ASN:O	1:A:41:VAL:HG12	2.14	0.47
1:A:104:ARG:HH21	1:A:104:ARG:HG2	1.78	0.47
1:A:94:VAL:HG23	1:A:95:GLN:N	2.30	0.46
1:A:1:MSE:HB2	1:A:100:ASP:O	2.16	0.46
1:A:161:ASN:O	1:A:165:LYS:HB2	2.17	0.45
1:A:34:GLY:HA3	1:A:80:TYR:CG	2.52	0.44
1:A:119:ASP:C	1:A:121:LEU:H	2.20	0.44
1:A:154:HIS:HB2	3:A:202:HOH:O	2.16	0.44
1:A:47:PRO:HG2	1:A:50:GLU:CG	2.47	0.43
1:A:13:VAL:HG21	1:A:108:LEU:O	2.19	0.43
1:A:2:LYS:N	1:A:2:LYS:HD3	2.34	0.42
1:A:138:GLU:O	1:A:142:LYS:HG2	2.19	0.42
1:A:173:PHE:C	1:A:175:PHE:N	2.72	0.42
1:A:117:ARG:HA	1:A:117:ARG:HD3	1.85	0.41
1:A:122:ARG:HG3	1:A:123:LYS:N	2.35	0.41
1:A:110:THR:C	1:A:153:SER:HB3	2.40	0.41
1:A:41:VAL:HG13	1:A:45:TYR:CD1	2.42	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	168/189 (89%)	159 (95%)	7 (4%)	2 (1%)	11 16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ILE
1	A	123	LYS

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	152/163 (93%)	150 (99%)	2 (1%)	65 81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	147	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	38	ASN
1	A	61	ASN
1	A	68	ASN
1	A	74	ASN
1	A	92	GLN
1	A	159	ASN
1	A	161	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 oligosaccharides 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	SO4	A	190	-	4,4,4	0.35	0	6,6,6	0.05	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, 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	170/189 (89%)	0.43	15 (8%)	17	16	6, 23, 51, 57	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	CYS	4.2
1	A	132	CYS	4.0
1	A	116	LEU	3.5
1	A	117	ARG	3.5
1	A	130	GLU	2.9
1	A	120	ALA	2.9
1	A	121	LEU	2.8
1	A	174	ILE	2.7
1	A	167	LEU	2.6
1	A	175	PHE	2.4
1	A	131	ARG	2.4
1	A	134	GLU	2.2
1	A	49	TRP	2.1
1	A	122	ARG	2.1
1	A	123	LYS	2.0

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	SO4	A	190	5/5	0.97	0.06	21,21,22,22	0

6.5 Other polymers

There are no such residues in this entry.