W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 23, 2021 – 05:23 PM EST

PDB ID	:	2IA1
Title	:	Crystal structure of protein BH3703 from Bacillus halodurans, Pfam DUF600
Authors	:	Ramagopal, U.A.; Russell, M.; Toro, R.; Freeman, J.C.; Reyes, C.; Gheyi, T.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2006-09-06
Resolution	:	1.59 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

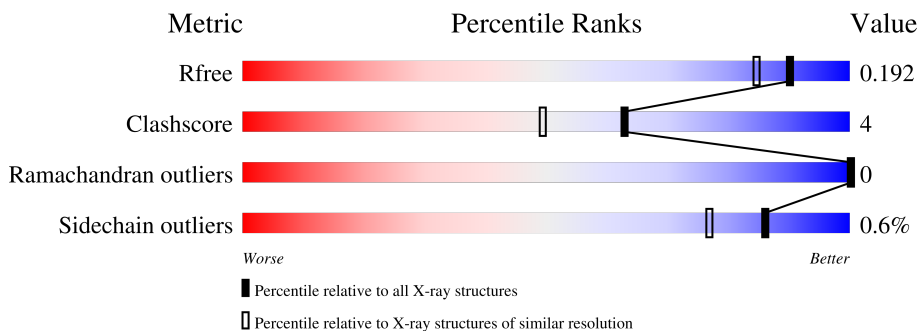|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 1.59 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	Percentile Ranks	Value
Rfree		0.192
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		0.6%

Worse ——— *Better*

▌ Percentile relative to all X-ray structures

⧘ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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	178	87% 8% · 5%
1	B	178	86% 9% · ·

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
3	GOL	B	602	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3681 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 BH3703 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total 1624	C 1060	N 249	O 308	S 7	0	18	0
1	B	170	Total 1601	C 1046	N 248	O 300	S 7	0	14	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	cloning artifact	UNP Q9K6M5
A	1	LEU	-	cloning artifact	UNP Q9K6M5
A	170	GLU	-	cloning artifact	UNP Q9K6M5
A	171	GLY	-	cloning artifact	UNP Q9K6M5
A	172	HIS	-	expression tag	UNP Q9K6M5
A	173	HIS	-	expression tag	UNP Q9K6M5
A	174	HIS	-	expression tag	UNP Q9K6M5
A	175	HIS	-	expression tag	UNP Q9K6M5
A	176	HIS	-	expression tag	UNP Q9K6M5
A	177	HIS	-	expression tag	UNP Q9K6M5
B	0	SER	-	cloning artifact	UNP Q9K6M5
B	1	LEU	-	cloning artifact	UNP Q9K6M5
B	170	GLU	-	cloning artifact	UNP Q9K6M5
B	171	GLY	-	cloning artifact	UNP Q9K6M5
B	172	HIS	-	expression tag	UNP Q9K6M5
B	173	HIS	-	expression tag	UNP Q9K6M5
B	174	HIS	-	expression tag	UNP Q9K6M5
B	175	HIS	-	expression tag	UNP Q9K6M5
B	176	HIS	-	expression tag	UNP Q9K6M5
B	177	HIS	-	expression tag	UNP Q9K6M5

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

SO4

O1

O3 O⁻ — S — O⁻ O4

S

O2

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1   C2

HO   OH

O1   O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

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PROTEIN DATA BANK

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	227	Total 227	O 227	0	0
4	B	212	Total 212	O 212	0	0

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. 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: BH3703 protein

Chain A:
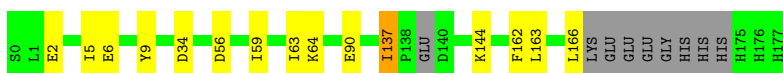
• Molecule 1: BH3703 protein

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.39Å 81.45Å 91.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.75 – 1.59	Depositor
	46.26 – 1.59	EDS
% Data completeness (in resolution range)	99.2 (60.75-1.59)	Depositor
	99.2 (46.26-1.59)	EDS
R_{merge}	0.04	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	4.08 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.172 , 0.192	Depositor
	0.172 , 0.192	DCC
R_{free} test set	3592 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 43.4	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3681	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GOL, 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	0.99	0/1677	0.84	1/2263 (0.0%)
1	B	0.93	0/1655	0.88	4/2230 (0.2%)
All	All	0.96	0/3332	0.86	5/4493 (0.1%)

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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	56	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	B	121	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	56	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	B	60	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	85	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ILE	Peptide

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	1624	0	1474	13	0
1	B	1601	0	1458	14	0
2	A	5	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	4	0
4	A	227	0	0	4	0
4	B	212	0	0	4	0
All	All	3681	0	2948	27	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 4.

The worst 5 of 27 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:2:GLU:O	1:A:6[B]:GLU:HG2	1.56	1.05
1:A:59:ILE:HG22	1:A:63[B]:ILE:HD13	1.61	0.82
1:B:70:PHE:HD1	3:B:602:GOL:H11	1.55	0.70
1:A:63[B]:ILE:HD11	4:A:640:HOH:O	1.95	0.67
1:A:90[A]:GLU:HG3	4:A:752:HOH:O	1.97	0.65

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	181/178 (102%)	181 (100%)	0	0	100	100
1	B	178/178 (100%)	177 (99%)	1 (1%)	0	100	100
All	All	359/356 (101%)	358 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	173/163 (106%)	171 (99%)	2 (1%)	71	54
1	B	170/163 (104%)	170 (100%)	0	100	100
All	All	343/326 (105%)	341 (99%)	2 (1%)	86	77

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

Mol	Chain	Res	Type
1	A	9	TYR
1	A	144	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	SO4	A	603	-	4,4,4	0.20	0	6,6,6	0.41	0
3	GOL	B	602	-	5,5,5	0.81	0	5,5,5	0.66	0
3	GOL	A	601	-	5,5,5	0.66	0	5,5,5	0.61	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
3	GOL	B	602	-	-	2/4/4/4	-
3	GOL	A	601	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	GOL	O1-C1-C2-O2
3	B	602	GOL	O1-C1-C2-C3
3	A	601	GOL	C1-C2-C3-O3
3	A	601	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	GOL	4	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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