wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2023 – 09:48 PM EDT

PDB ID	:	2QEE
Title	:	Crystal structure of putative amidohydrolase BH0493 from Bacillus halodurans C-125
Authors	:	Malashkevich, V.N.; Toro, R.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-06-25
Resolution	:	1.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

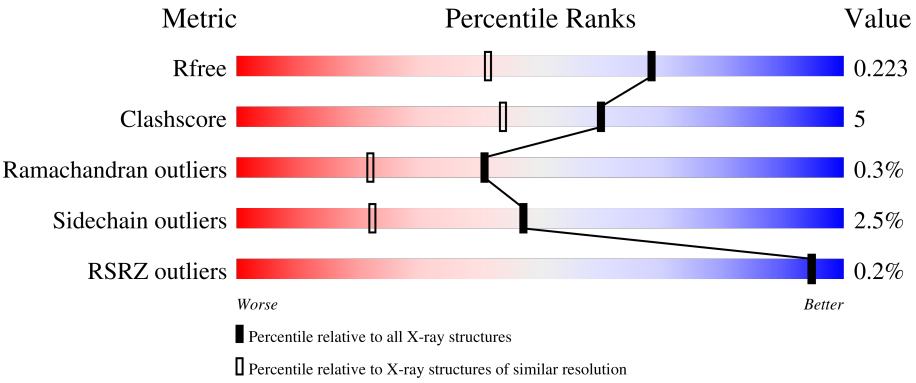
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	437	87% 7% • 5%
1	B	437	86% 8% •• 5%
1	C	437	86% 8% • 5%
1	D	437	86% 8% • 5%
1	E	437	87% 9% • •

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Mol	Chain	Length	Quality of chain
1	F	437	
1	G	437	
1	H	437	
1	I	437	
1	J	437	
1	K	437	
1	L	437	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 46314 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 BH0493 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	7	0
			3464	2209	600	635	20			
1	B	415	Total	C	N	O	S	0	2	0
			3428	2185	591	632	20			
1	C	417	Total	C	N	O	S	0	7	0
			3474	2213	600	641	20			
1	D	415	Total	C	N	O	S	0	4	0
			3444	2196	596	632	20			
1	E	424	Total	C	N	O	S	0	5	0
			3519	2242	611	646	20			
1	F	416	Total	C	N	O	S	0	4	0
			3447	2199	594	634	20			
1	G	415	Total	C	N	O	S	0	0	0
			3420	2180	591	629	20			
1	H	416	Total	C	N	O	S	0	3	0
			3443	2194	595	634	20			
1	I	416	Total	C	N	O	S	0	5	0
			3453	2202	598	633	20			
1	J	414	Total	C	N	O	S	0	0	0
			3412	2176	589	627	20			
1	K	414	Total	C	N	O	S	0	3	0
			3419	2181	586	632	20			
1	L	418	Total	C	N	O	S	0	1	0
			3450	2197	597	636	20			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP Q9KFI6
A	0	SER	-	cloning artifact	UNP Q9KFI6
A	1	LEU	-	cloning artifact	UNP Q9KFI6
A	428	GLU	-	cloning artifact	UNP Q9KFI6
A	429	GLY	-	cloning artifact	UNP Q9KFI6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	430	HIS	-	cloning artifact	UNP Q9KFI6
A	431	HIS	-	cloning artifact	UNP Q9KFI6
A	432	HIS	-	cloning artifact	UNP Q9KFI6
A	433	HIS	-	cloning artifact	UNP Q9KFI6
A	434	HIS	-	cloning artifact	UNP Q9KFI6
A	435	HIS	-	cloning artifact	UNP Q9KFI6
B	-1	MET	-	cloning artifact	UNP Q9KFI6
B	0	SER	-	cloning artifact	UNP Q9KFI6
B	1	LEU	-	cloning artifact	UNP Q9KFI6
B	428	GLU	-	cloning artifact	UNP Q9KFI6
B	429	GLY	-	cloning artifact	UNP Q9KFI6
B	430	HIS	-	cloning artifact	UNP Q9KFI6
B	431	HIS	-	cloning artifact	UNP Q9KFI6
B	432	HIS	-	cloning artifact	UNP Q9KFI6
B	433	HIS	-	cloning artifact	UNP Q9KFI6
B	434	HIS	-	cloning artifact	UNP Q9KFI6
B	435	HIS	-	cloning artifact	UNP Q9KFI6
C	-1	MET	-	cloning artifact	UNP Q9KFI6
C	0	SER	-	cloning artifact	UNP Q9KFI6
C	1	LEU	-	cloning artifact	UNP Q9KFI6
C	428	GLU	-	cloning artifact	UNP Q9KFI6
C	429	GLY	-	cloning artifact	UNP Q9KFI6
C	430	HIS	-	cloning artifact	UNP Q9KFI6
C	431	HIS	-	cloning artifact	UNP Q9KFI6
C	432	HIS	-	cloning artifact	UNP Q9KFI6
C	433	HIS	-	cloning artifact	UNP Q9KFI6
C	434	HIS	-	cloning artifact	UNP Q9KFI6
C	435	HIS	-	cloning artifact	UNP Q9KFI6
D	-1	MET	-	cloning artifact	UNP Q9KFI6
D	0	SER	-	cloning artifact	UNP Q9KFI6
D	1	LEU	-	cloning artifact	UNP Q9KFI6
D	428	GLU	-	cloning artifact	UNP Q9KFI6
D	429	GLY	-	cloning artifact	UNP Q9KFI6
D	430	HIS	-	cloning artifact	UNP Q9KFI6
D	431	HIS	-	cloning artifact	UNP Q9KFI6
D	432	HIS	-	cloning artifact	UNP Q9KFI6
D	433	HIS	-	cloning artifact	UNP Q9KFI6
D	434	HIS	-	cloning artifact	UNP Q9KFI6
D	435	HIS	-	cloning artifact	UNP Q9KFI6
E	-1	MET	-	cloning artifact	UNP Q9KFI6
E	0	SER	-	cloning artifact	UNP Q9KFI6
E	1	LEU	-	cloning artifact	UNP Q9KFI6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	428	GLU	-	cloning artifact	UNP Q9KFI6
E	429	GLY	-	cloning artifact	UNP Q9KFI6
E	430	HIS	-	cloning artifact	UNP Q9KFI6
E	431	HIS	-	cloning artifact	UNP Q9KFI6
E	432	HIS	-	cloning artifact	UNP Q9KFI6
E	433	HIS	-	cloning artifact	UNP Q9KFI6
E	434	HIS	-	cloning artifact	UNP Q9KFI6
E	435	HIS	-	cloning artifact	UNP Q9KFI6
F	-1	MET	-	cloning artifact	UNP Q9KFI6
F	0	SER	-	cloning artifact	UNP Q9KFI6
F	1	LEU	-	cloning artifact	UNP Q9KFI6
F	428	GLU	-	cloning artifact	UNP Q9KFI6
F	429	GLY	-	cloning artifact	UNP Q9KFI6
F	430	HIS	-	cloning artifact	UNP Q9KFI6
F	431	HIS	-	cloning artifact	UNP Q9KFI6
F	432	HIS	-	cloning artifact	UNP Q9KFI6
F	433	HIS	-	cloning artifact	UNP Q9KFI6
F	434	HIS	-	cloning artifact	UNP Q9KFI6
F	435	HIS	-	cloning artifact	UNP Q9KFI6
G	-1	MET	-	cloning artifact	UNP Q9KFI6
G	0	SER	-	cloning artifact	UNP Q9KFI6
G	1	LEU	-	cloning artifact	UNP Q9KFI6
G	428	GLU	-	cloning artifact	UNP Q9KFI6
G	429	GLY	-	cloning artifact	UNP Q9KFI6
G	430	HIS	-	cloning artifact	UNP Q9KFI6
G	431	HIS	-	cloning artifact	UNP Q9KFI6
G	432	HIS	-	cloning artifact	UNP Q9KFI6
G	433	HIS	-	cloning artifact	UNP Q9KFI6
G	434	HIS	-	cloning artifact	UNP Q9KFI6
G	435	HIS	-	cloning artifact	UNP Q9KFI6
H	-1	MET	-	cloning artifact	UNP Q9KFI6
H	0	SER	-	cloning artifact	UNP Q9KFI6
H	1	LEU	-	cloning artifact	UNP Q9KFI6
H	428	GLU	-	cloning artifact	UNP Q9KFI6
H	429	GLY	-	cloning artifact	UNP Q9KFI6
H	430	HIS	-	cloning artifact	UNP Q9KFI6
H	431	HIS	-	cloning artifact	UNP Q9KFI6
H	432	HIS	-	cloning artifact	UNP Q9KFI6
H	433	HIS	-	cloning artifact	UNP Q9KFI6
H	434	HIS	-	cloning artifact	UNP Q9KFI6
H	435	HIS	-	cloning artifact	UNP Q9KFI6
I	-1	MET	-	cloning artifact	UNP Q9KFI6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	0	SER	-	cloning artifact	UNP Q9KFI6
I	1	LEU	-	cloning artifact	UNP Q9KFI6
I	428	GLU	-	cloning artifact	UNP Q9KFI6
I	429	GLY	-	cloning artifact	UNP Q9KFI6
I	430	HIS	-	cloning artifact	UNP Q9KFI6
I	431	HIS	-	cloning artifact	UNP Q9KFI6
I	432	HIS	-	cloning artifact	UNP Q9KFI6
I	433	HIS	-	cloning artifact	UNP Q9KFI6
I	434	HIS	-	cloning artifact	UNP Q9KFI6
I	435	HIS	-	cloning artifact	UNP Q9KFI6
J	-1	MET	-	cloning artifact	UNP Q9KFI6
J	0	SER	-	cloning artifact	UNP Q9KFI6
J	1	LEU	-	cloning artifact	UNP Q9KFI6
J	428	GLU	-	cloning artifact	UNP Q9KFI6
J	429	GLY	-	cloning artifact	UNP Q9KFI6
J	430	HIS	-	cloning artifact	UNP Q9KFI6
J	431	HIS	-	cloning artifact	UNP Q9KFI6
J	432	HIS	-	cloning artifact	UNP Q9KFI6
J	433	HIS	-	cloning artifact	UNP Q9KFI6
J	434	HIS	-	cloning artifact	UNP Q9KFI6
J	435	HIS	-	cloning artifact	UNP Q9KFI6
K	-1	MET	-	cloning artifact	UNP Q9KFI6
K	0	SER	-	cloning artifact	UNP Q9KFI6
K	1	LEU	-	cloning artifact	UNP Q9KFI6
K	428	GLU	-	cloning artifact	UNP Q9KFI6
K	429	GLY	-	cloning artifact	UNP Q9KFI6
K	430	HIS	-	cloning artifact	UNP Q9KFI6
K	431	HIS	-	cloning artifact	UNP Q9KFI6
K	432	HIS	-	cloning artifact	UNP Q9KFI6
K	433	HIS	-	cloning artifact	UNP Q9KFI6
K	434	HIS	-	cloning artifact	UNP Q9KFI6
K	435	HIS	-	cloning artifact	UNP Q9KFI6
L	-1	MET	-	cloning artifact	UNP Q9KFI6
L	0	SER	-	cloning artifact	UNP Q9KFI6
L	1	LEU	-	cloning artifact	UNP Q9KFI6
L	428	GLU	-	cloning artifact	UNP Q9KFI6
L	429	GLY	-	cloning artifact	UNP Q9KFI6
L	430	HIS	-	cloning artifact	UNP Q9KFI6
L	431	HIS	-	cloning artifact	UNP Q9KFI6
L	432	HIS	-	cloning artifact	UNP Q9KFI6
L	433	HIS	-	cloning artifact	UNP Q9KFI6
L	434	HIS	-	cloning artifact	UNP Q9KFI6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	435	HIS	-	cloning artifact	UNP Q9KFI6

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	2	Total Cl 2 2	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	G	2	Total Cl 2 2	0	0
2	H	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	J	2	Total Cl 2 2	0	0
2	K	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	G	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0
4	I	1	Total Zn 1 1	0	0
4	J	1	Total Zn 1 1	0	0
4	K	1	Total Zn 1 1	0	0
4	L	1	Total Zn 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	435	Total O 435 435	0	0
5	B	450	Total O 450 450	0	0
5	C	459	Total O 459 459	0	0
5	D	423	Total O 423 423	0	0
5	E	452	Total O 452 452	0	0
5	F	432	Total O 432 432	0	0
5	G	394	Total O 394 394	0	0
5	H	439	Total O 439 439	0	0

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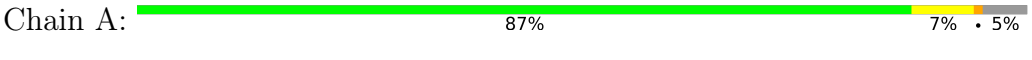
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	386	Total O 386 386	0	0
5	J	348	Total O 348 348	0	0
5	K	344	Total O 344 344	0	0
5	L	347	Total O 347 347	0	0

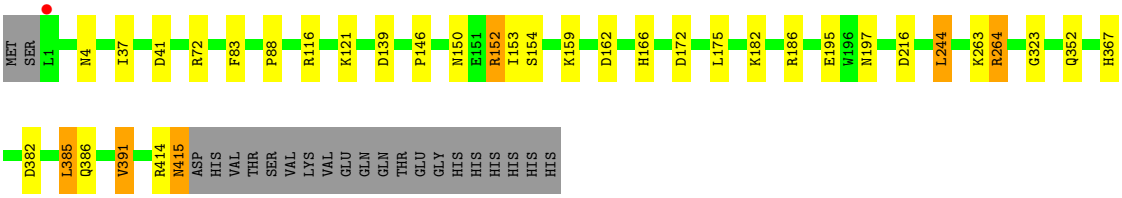
3 Residue-property plots (i)

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: BH0493 protein

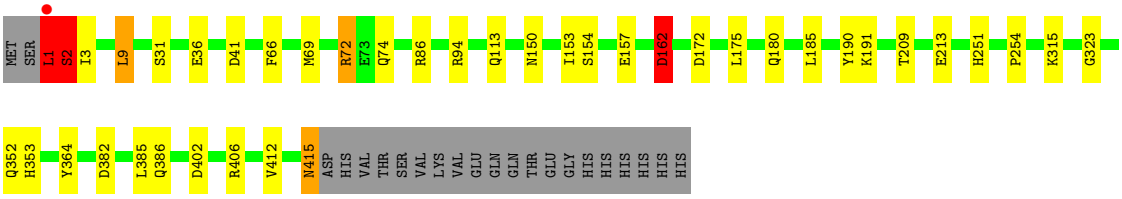
Chain A:





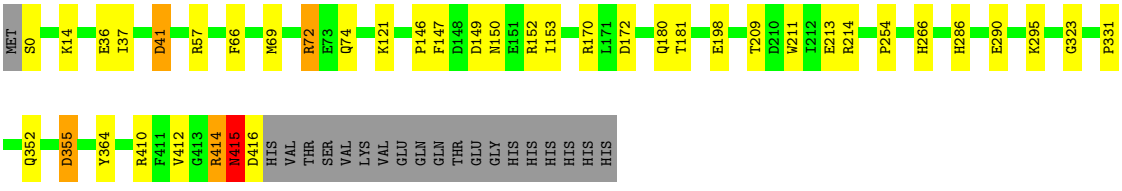
- Molecule 1: BH0493 protein

Chain B:



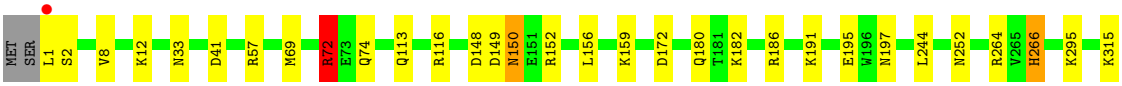
- Molecule 1: BH0493 protein

Chain C:



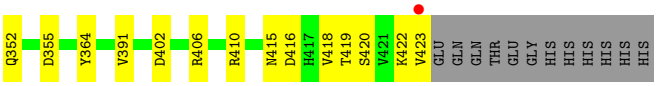
- Molecule 1: BH0493 protein

Chain D:



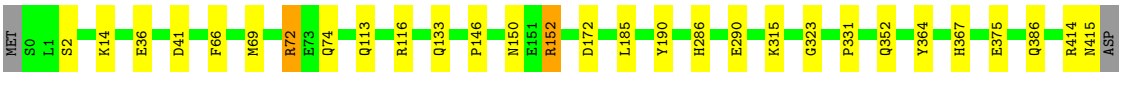
• Molecule 1: BH0493 protein

Chain E:



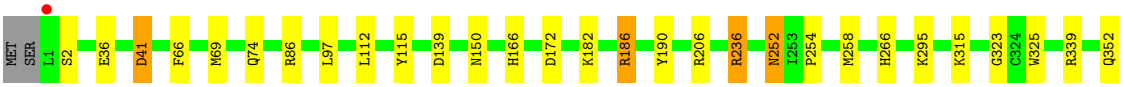
• Molecule 1: BH0493 protein

Chain F:



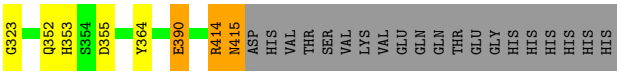
• Molecule 1: BH0493 protein

Chain G:



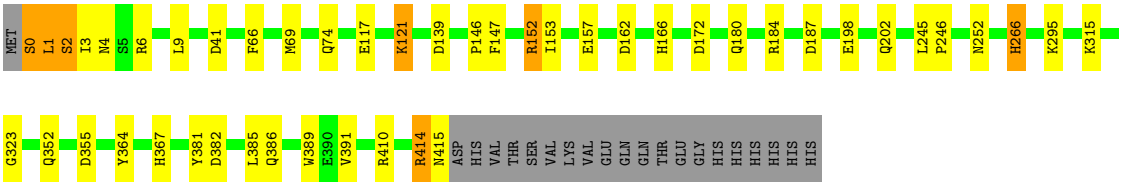
• Molecule 1: BH0493 protein

Chain H:



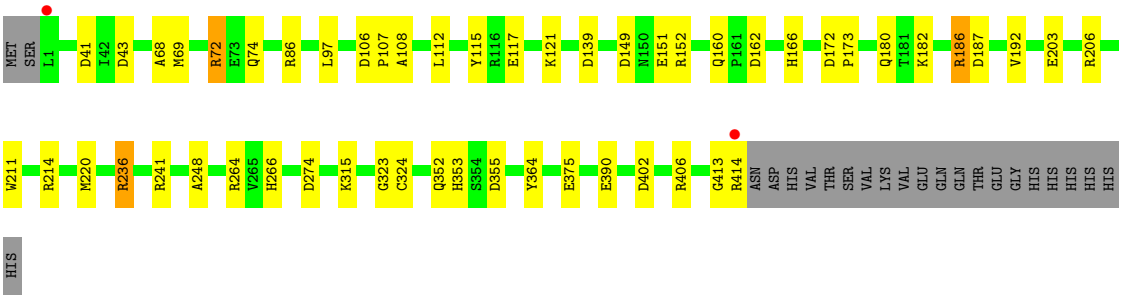
• Molecule 1: BH0493 protein

Chain I:



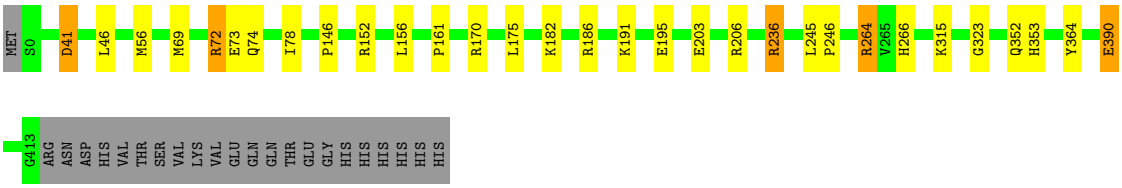
• Molecule 1: BH0493 protein

Chain J:



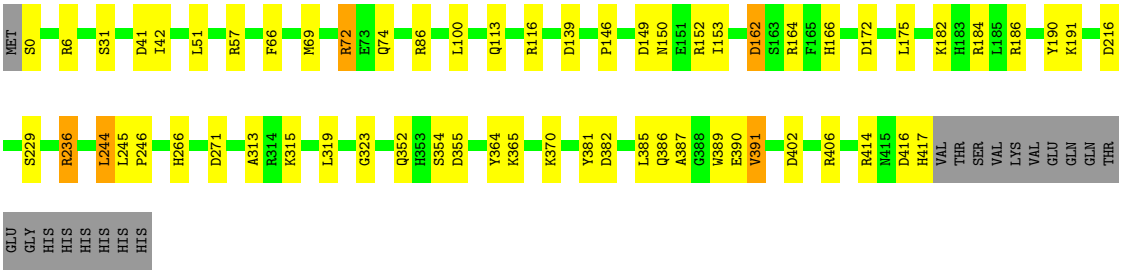
• Molecule 1: BH0493 protein

Chain K:



• Molecule 1: BH0493 protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	122.00Å 122.21Å 127.58Å 78.85° 78.95° 80.92°	Depositor
Resolution (Å)	19.99 – 1.65 19.97 – 1.65	Depositor EDS
% Data completeness (in resolution range)	89.6 (19.99-1.65) 89.4 (19.97-1.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.64 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.224 0.187 , 0.223	Depositor DCC
R_{free} test set	37962 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,l,h 0.013 for l,h,k 0.178 for -k,-h,-l 0.016 for -l,-k,-h 0.014 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	46314	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9124e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MG, ZN, CL

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	0.86	0/3570	0.83	2/4835 (0.0%)
1	B	0.85	0/3518	0.85	5/4767 (0.1%)
1	C	0.93	1/3579 (0.0%)	0.87	2/4847 (0.0%)
1	D	0.82	0/3541	0.80	1/4797 (0.0%)
1	E	0.89	0/3620	0.90	4/4904 (0.1%)
1	F	0.88	0/3544	0.82	0/4802
1	G	0.80	0/3504	0.80	3/4748 (0.1%)
1	H	0.88	1/3536 (0.0%)	0.83	1/4790 (0.0%)
1	I	0.82	0/3553	0.78	0/4812
1	J	0.79	1/3496 (0.0%)	0.78	1/4737 (0.0%)
1	K	0.75	0/3512	0.77	2/4759 (0.0%)
1	L	0.75	0/3538	0.78	3/4794 (0.1%)
All	All	0.84	3/42511 (0.0%)	0.82	24/57592 (0.0%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	11	GLU	CG-CD	5.35	1.59	1.51
1	J	324	CYS	CB-SG	-5.06	1.73	1.81
1	C	355	ASP	CB-CG	-5.05	1.41	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	236	ARG	NE-CZ-NH1	17.65	129.13	120.30
1	E	236	ARG	NE-CZ-NH2	-15.97	112.32	120.30
1	L	236	ARG	NE-CZ-NH2	-11.34	114.63	120.30
1	L	236	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	G	236	ARG	NE-CZ-NH2	-7.27	116.66	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	SER	Peptide

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	3464	0	3406	27	0
1	B	3428	0	3357	27	0
1	C	3474	0	3413	33	0
1	D	3444	0	3379	39	0
1	E	3519	0	3460	29	0
1	F	3447	0	3382	35	0
1	G	3420	0	3348	25	0
1	H	3443	0	3377	27	0
1	I	3453	0	3396	44	0
1	J	3412	0	3342	38	0
1	K	3419	0	3350	24	0
1	L	3450	0	3372	45	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	435	0	0	5	0
5	B	450	0	0	4	0
5	C	459	0	0	10	0
5	D	423	0	0	13	0
5	E	452	0	0	11	0
5	F	432	0	0	7	0
5	G	394	0	0	8	0
5	H	439	0	0	9	0
5	I	386	0	0	14	0
5	J	348	0	0	8	0
5	K	344	0	0	7	0
5	L	347	0	0	5	0
All	All	46314	0	40582	378	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 5.

The worst 5 of 378 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:F:152:ARG:HH21	1:F:152:ARG:CB	1.51	1.23
1:J:413:GLY:HA2	1:J:414:ARG:HB2	1.24	1.18
1:G:391:VAL:HB	5:G:5223:HOH:O	1.40	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:VAL:HB	5:E:5194:HOH:O	1.43	1.16
1:F:152:ARG:HH21	1:F:152:ARG:HB3	1.03	1.14

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	420/437 (96%)	413 (98%)	6 (1%)	1 (0%)	47	28
1	B	415/437 (95%)	405 (98%)	8 (2%)	2 (0%)	29	11
1	C	422/437 (97%)	414 (98%)	6 (1%)	2 (0%)	29	11
1	D	417/437 (95%)	408 (98%)	8 (2%)	1 (0%)	47	28
1	E	427/437 (98%)	418 (98%)	7 (2%)	2 (0%)	29	11
1	F	418/437 (96%)	413 (99%)	4 (1%)	1 (0%)	47	28
1	G	413/437 (94%)	405 (98%)	7 (2%)	1 (0%)	47	28
1	H	417/437 (95%)	408 (98%)	8 (2%)	1 (0%)	47	28
1	I	419/437 (96%)	408 (97%)	9 (2%)	2 (0%)	29	11
1	J	412/437 (94%)	403 (98%)	7 (2%)	2 (0%)	29	11
1	K	415/437 (95%)	405 (98%)	9 (2%)	1 (0%)	47	28
1	L	417/437 (95%)	407 (98%)	9 (2%)	1 (0%)	47	28
All	All	5012/5244 (96%)	4907 (98%)	88 (2%)	17 (0%)	41	22

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	B	2	SER
1	B	41	ASP

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Mol	Chain	Res	Type
1	C	41	ASP
1	C	415	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	382/396 (96%)	371 (97%)	11 (3%)	42	16
1	B	377/396 (95%)	365 (97%)	12 (3%)	39	13
1	C	384/396 (97%)	375 (98%)	9 (2%)	50	25
1	D	379/396 (96%)	369 (97%)	10 (3%)	46	21
1	E	389/396 (98%)	377 (97%)	12 (3%)	40	14
1	F	380/396 (96%)	375 (99%)	5 (1%)	69	50
1	G	375/396 (95%)	366 (98%)	9 (2%)	49	23
1	H	379/396 (96%)	369 (97%)	10 (3%)	46	21
1	I	381/396 (96%)	369 (97%)	12 (3%)	40	14
1	J	374/396 (94%)	367 (98%)	7 (2%)	57	34
1	K	377/396 (95%)	370 (98%)	7 (2%)	57	34
1	L	379/396 (96%)	368 (97%)	11 (3%)	42	16
All	All	4556/4752 (96%)	4441 (98%)	115 (2%)	47	22

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	331	PRO
1	L	229	SER
1	H	264[B]	ARG
1	L	175	LEU
1	K	191	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	49	HIS
1	J	266	HIS
1	I	202	GLN
1	J	15	ASN
1	K	193	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 32 are monoatomic - 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

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

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	415/437 (94%)	-0.95	1 (0%) 95 95	12, 21, 44, 68	0
1	B	415/437 (94%)	-0.96	1 (0%) 95 95	12, 21, 39, 60	0
1	C	417/437 (95%)	-0.95	0 100 100	11, 19, 38, 67	0
1	D	415/437 (94%)	-0.96	1 (0%) 95 95	13, 23, 44, 64	0
1	E	424/437 (97%)	-0.93	2 (0%) 91 92	11, 21, 40, 70	0
1	F	416/437 (95%)	-0.96	0 100 100	12, 21, 42, 61	0
1	G	415/437 (94%)	-0.88	1 (0%) 95 95	13, 25, 48, 66	0
1	H	416/437 (95%)	-0.96	0 100 100	13, 22, 38, 64	0
1	I	416/437 (95%)	-0.94	0 100 100	13, 24, 44, 64	0
1	J	414/437 (94%)	-0.81	2 (0%) 91 92	16, 29, 51, 68	0
1	K	414/437 (94%)	-0.86	0 100 100	15, 27, 49, 63	0
1	L	418/437 (95%)	-0.90	0 100 100	15, 28, 50, 68	0
All	All	4995/5244 (95%)	-0.92	8 (0%) 95 95	11, 23, 45, 70	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	LEU	6.1
1	D	1	LEU	5.6
1	B	1	LEU	5.0
1	E	423	VAL	4.1
1	J	1	LEU	3.8

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 (i)

There are no monosaccharides 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, 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
4	ZN	K	5031	1/1	0.98	0.03	39,39,39,39	1
2	CL	G	5007	1/1	0.99	0.08	28,28,28,28	0
2	CL	H	5013	1/1	0.99	0.06	28,28,28,28	0
2	CL	J	5012	1/1	0.99	0.07	32,32,32,32	0
2	CL	K	5014	1/1	0.99	0.06	30,30,30,30	0
2	CL	L	5015	1/1	0.99	0.05	32,32,32,32	0
4	ZN	B	5022	1/1	0.99	0.03	35,35,35,35	1
4	ZN	D	5024	1/1	0.99	0.03	36,36,36,36	1
4	ZN	E	5025	1/1	0.99	0.03	35,35,35,35	1
4	ZN	G	5027	1/1	0.99	0.03	40,40,40,40	1
4	ZN	I	5029	1/1	0.99	0.03	34,34,34,34	1
2	CL	F	5016	1/1	0.99	0.06	27,27,27,27	0
4	ZN	L	5032	1/1	0.99	0.03	35,35,35,35	1
2	CL	C	5011	1/1	1.00	0.05	25,25,25,25	0
2	CL	D	5002	1/1	1.00	0.07	14,14,14,14	0
2	CL	D	5005	1/1	1.00	0.08	27,27,27,27	0
3	MG	A	5018	1/1	1.00	0.04	14,14,14,14	0
3	MG	D	5019	1/1	1.00	0.05	15,15,15,15	0
3	MG	G	5017	1/1	1.00	0.05	15,15,15,15	0
3	MG	J	5020	1/1	1.00	0.06	18,18,18,18	0
4	ZN	A	5021	1/1	1.00	0.03	36,36,36,36	1
2	CL	E	5008	1/1	1.00	0.07	24,24,24,24	0
4	ZN	C	5023	1/1	1.00	0.03	30,30,30,30	1
2	CL	A	5001	1/1	1.00	0.08	13,13,13,13	0
2	CL	G	5003	1/1	1.00	0.07	14,14,14,14	0
4	ZN	F	5026	1/1	1.00	0.03	31,31,31,31	1
2	CL	A	5006	1/1	1.00	0.08	27,27,27,27	0
4	ZN	H	5028	1/1	1.00	0.03	31,31,31,31	1
2	CL	B	5010	1/1	1.00	0.06	24,24,24,24	0
4	ZN	J	5030	1/1	1.00	0.02	38,38,38,38	1
2	CL	I	5009	1/1	1.00	0.07	26,26,26,26	0
2	CL	J	5004	1/1	1.00	0.07	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.