



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 07:28 PM GMT

PDB ID : 2Q08
Title : Crystal structure of the protein BH0493 from Bacillus halodurans C-125 complexed with ZN
Authors : Fedorov, A.A.; Fedorov, E.V.; Patskovsky, Y.; Sauder, J.M.; Burley, S.K.; Raushel, F.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-05-21
Resolution : 2.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

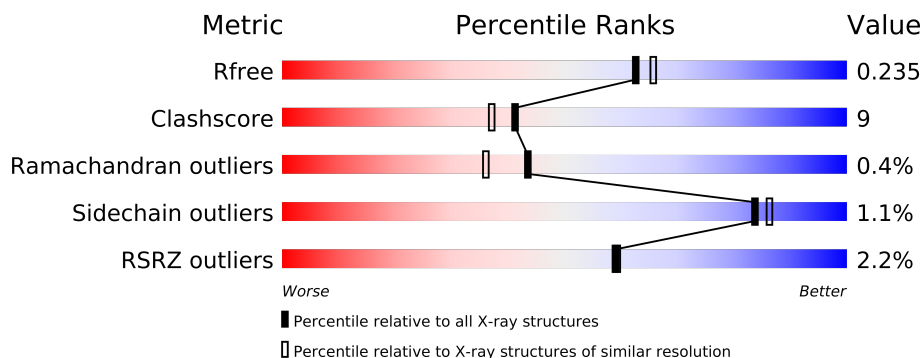
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 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}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	427	
1	B	427	
1	C	427	
1	D	427	
1	E	427	
1	F	427	
1	G	427	
1	H	427	
1	I	427	
1	J	427	
1	K	427	
1	L	427	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41791 atoms, of which 0 are hydrogen and 0 are deuterium.

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	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			
1	B	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			
1	C	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			
1	D	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			
1	E	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			
1	F	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			
1	G	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			
1	H	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			
1	I	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			
1	J	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			
1	K	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			
1	L	413	Total	C	N	O	S	0	0	0
			3401	2169	585	626	21			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	J	2	Total	Zn	0	0
			2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total 91	O 91	0	0
3	B	121	Total 121	O 121	0	0
3	C	84	Total 84	O 84	0	0
3	D	77	Total 77	O 77	0	0
3	E	73	Total 73	O 73	0	0
3	F	82	Total 82	O 82	0	0
3	G	79	Total 79	O 79	0	0
3	H	73	Total 73	O 73	0	0
3	I	83	Total 83	O 83	0	0

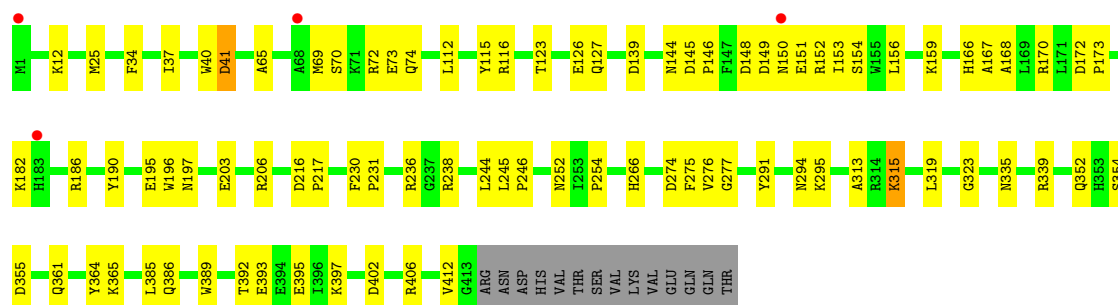
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	61	Total 61	O 61	0	0
3	K	70	Total 70	O 70	0	0
3	L	69	Total 69	O 69	0	0

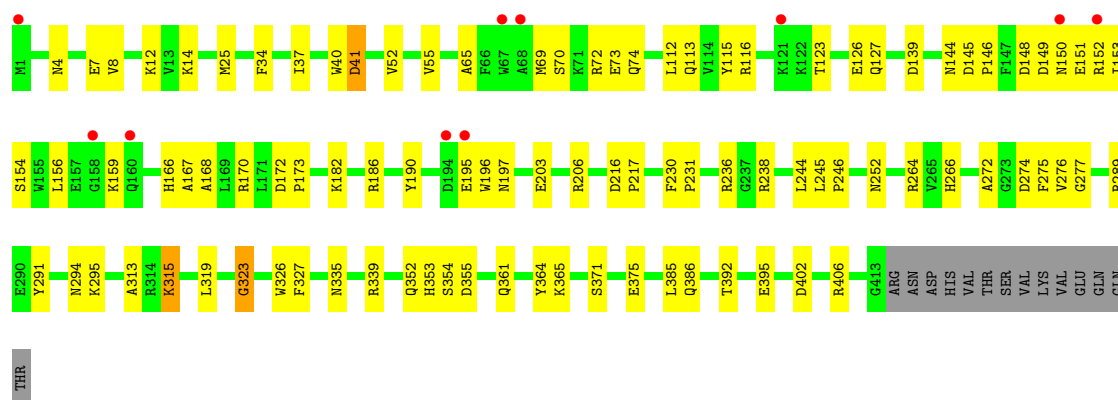
- Molecule 1: BH0493 protein

Chain D:



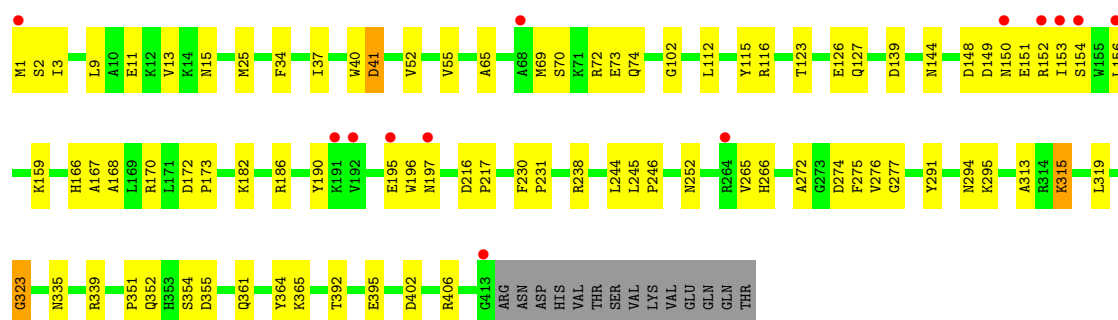
- Molecule 1: BH0493 protein

Chain E:



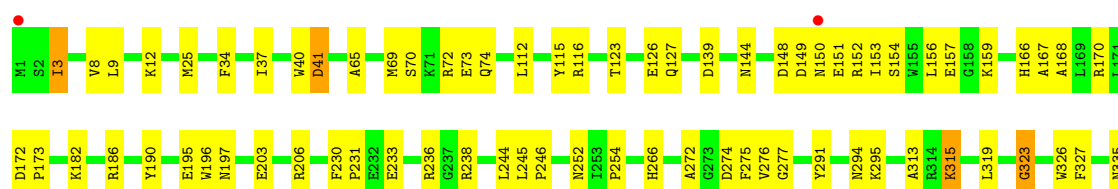
- Molecule 1: BH0493 protein

Chain F:



- Molecule 1: BH0493 protein

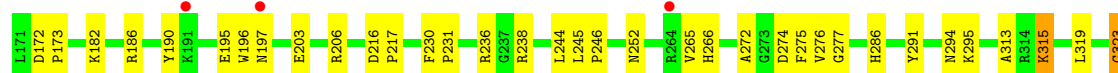
Chain G:





• Molecule 1: BH0493 protein

Chain H:



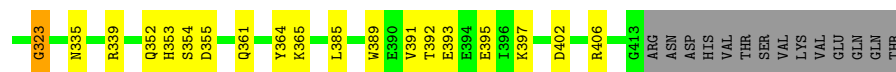
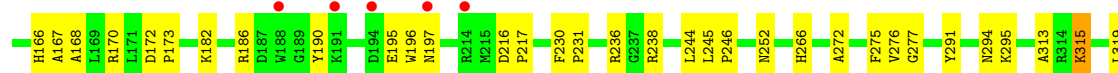
• Molecule 1: BH0493 protein

Chain I:



• Molecule 1: BH0493 protein

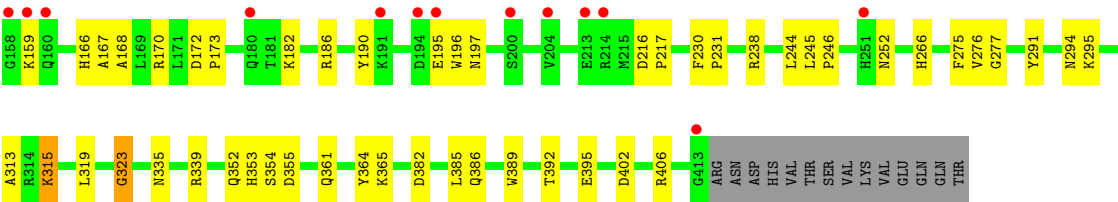
Chain J:



• Molecule 1: BH0493 protein

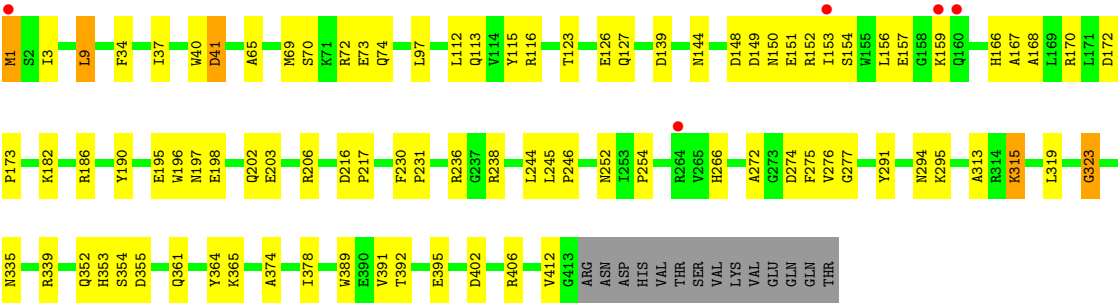
Chain K:





● Molecule 1: BH0493 protein

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	121.27Å 120.97Å 126.24Å 78.82° 78.67° 80.42°	Depositor
Resolution (Å)	24.93 – 2.00 39.39 – 1.98	Depositor EDS
% Data completeness (in resolution range)	90.1 (24.93-2.00) 88.7 (39.39-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.239 0.223 , 0.235	Depositor DCC
R_{free} test set	20880 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
Estimated twinning fraction	0.006 for l,h,k 0.006 for k,l,h 0.084 for -k,-h,-l 0.009 for -h,-l,-k 0.012 for -l,-k,-h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 451431 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41791	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 30.62 % 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 1.2677e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.35	0/3485	0.61	0/4722
1	B	0.36	0/3485	0.61	0/4722
1	C	0.36	0/3485	0.61	0/4722
1	D	0.35	0/3485	0.60	0/4722
1	E	0.35	0/3485	0.60	0/4722
1	F	0.35	0/3485	0.61	0/4722
1	G	0.35	0/3485	0.60	0/4722
1	H	0.34	0/3485	0.60	0/4722
1	I	0.35	0/3485	0.60	0/4722
1	J	0.34	0/3485	0.60	0/4722
1	K	0.34	0/3485	0.60	0/4722
1	L	0.35	0/3485	0.60	0/4722
All	All	0.35	0/41820	0.60	0/56664

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3401	0	3327	65	0
1	B	3401	0	3327	66	2
1	C	3401	0	3327	79	0
1	D	3401	0	3327	61	0
1	E	3401	0	3327	69	0
1	F	3401	0	3327	66	0
1	G	3401	0	3327	64	2
1	H	3401	0	3327	67	0
1	I	3401	0	3327	64	0
1	J	3401	0	3327	65	0
1	K	3401	0	3327	62	0
1	L	3401	0	3327	77	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	1	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	2	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	91	0	0	3	0
3	B	121	0	0	4	0
3	C	84	0	0	3	0
3	D	77	0	0	2	0
3	E	73	0	0	2	0
3	F	82	0	0	2	0
3	G	79	0	0	3	0
3	H	73	0	0	4	0
3	I	83	0	0	3	0
3	J	61	0	0	2	0
3	K	70	0	0	1	0
3	L	69	0	0	2	0
All	All	41791	0	39924	742	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 742 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:123:THR:OG1	1:L:198:GLU:HG2	1.41	1.18
1:G:152:ARG:HH12	1:L:157:GLU:HG2	1.05	1.14
1:G:152:ARG:NH1	1:L:157:GLU:HG2	1.65	1.11
1:C:8:VAL:O	1:C:12:LYS:HG2	1.57	1.04
1:E:40:TRP:O	1:E:41:ASP:HB2	1.58	1.04

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:194:ASP:OD2	1:G:233:GLU:N[1_455]	2.11	0.09
1:B:193:ASN:ND2	1:G:238:ARG:NH2[1_455]	2.17	0.03

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	411/427 (96%)	401 (98%)	9 (2%)	1 (0%)	56	51
1	B	411/427 (96%)	400 (97%)	10 (2%)	1 (0%)	56	51
1	C	411/427 (96%)	400 (97%)	10 (2%)	1 (0%)	56	51
1	D	411/427 (96%)	402 (98%)	8 (2%)	1 (0%)	56	51
1	E	411/427 (96%)	401 (98%)	8 (2%)	2 (0%)	38	29
1	F	411/427 (96%)	401 (98%)	8 (2%)	2 (0%)	38	29
1	G	411/427 (96%)	398 (97%)	10 (2%)	3 (1%)	30	20
1	H	411/427 (96%)	400 (97%)	9 (2%)	2 (0%)	38	29
1	I	411/427 (96%)	401 (98%)	7 (2%)	3 (1%)	30	20
1	J	411/427 (96%)	400 (97%)	9 (2%)	2 (0%)	38	29
1	K	411/427 (96%)	402 (98%)	7 (2%)	2 (0%)	38	29
1	L	411/427 (96%)	399 (97%)	10 (2%)	2 (0%)	38	29
All	All	4932/5124 (96%)	4805 (97%)	105 (2%)	22 (0%)	43	36

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	B	41	ASP
1	C	41	ASP
1	D	41	ASP
1	E	41	ASP

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	373/387 (96%)	369 (99%)	4 (1%)	84	86
1	B	373/387 (96%)	369 (99%)	4 (1%)	84	86
1	C	373/387 (96%)	368 (99%)	5 (1%)	80	82
1	D	373/387 (96%)	370 (99%)	3 (1%)	89	92
1	E	373/387 (96%)	368 (99%)	5 (1%)	80	82
1	F	373/387 (96%)	370 (99%)	3 (1%)	89	92
1	G	373/387 (96%)	369 (99%)	4 (1%)	84	86
1	H	373/387 (96%)	370 (99%)	3 (1%)	89	92
1	I	373/387 (96%)	369 (99%)	4 (1%)	84	86
1	J	373/387 (96%)	369 (99%)	4 (1%)	84	86
1	K	373/387 (96%)	370 (99%)	3 (1%)	89	92
1	L	373/387 (96%)	367 (98%)	6 (2%)	75	77
All	All	4476/4644 (96%)	4428 (99%)	48 (1%)	84	86

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	315	LYS
1	G	364	TYR
1	L	315	LYS
1	F	355	ASP
1	G	315	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	49	HIS
1	G	252	ASN
1	L	113	GLN
1	F	144	ASN
1	F	294	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 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.

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, 95th 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	413/427 (96%)	0.01	6 (1%) 70 70	17, 32, 53, 62	0
1	B	413/427 (96%)	-0.05	11 (2%) 52 52	16, 27, 51, 59	0
1	C	413/427 (96%)	-0.05	11 (2%) 52 52	17, 32, 54, 61	0
1	D	413/427 (96%)	0.04	4 (0%) 79 80	18, 33, 54, 61	0
1	E	413/427 (96%)	0.06	10 (2%) 56 56	19, 34, 54, 64	0
1	F	413/427 (96%)	0.07	13 (3%) 47 46	18, 33, 54, 62	0
1	G	413/427 (96%)	-0.08	2 (0%) 88 89	19, 32, 51, 58	0
1	H	413/427 (96%)	-0.04	7 (1%) 67 67	20, 33, 53, 60	0
1	I	413/427 (96%)	0.00	10 (2%) 56 56	19, 33, 54, 63	0
1	J	413/427 (96%)	0.08	13 (3%) 47 46	22, 38, 55, 61	0
1	K	413/427 (96%)	0.13	19 (4%) 31 30	22, 35, 56, 63	0
1	L	413/427 (96%)	-0.04	5 (1%) 75 76	19, 34, 54, 60	0
All	All	4956/5124 (96%)	0.01	111 (2%) 59 59	16, 33, 54, 64	0

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	8.0
1	J	1	MET	7.1
1	H	1	MET	7.0
1	G	1	MET	6.8
1	I	1	MET	6.7

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	H	995	1/1	0.11	-1.84	57,57,57,57	0
2	ZN	K	991	1/1	0.09	-2.23	66,66,66,66	0
2	ZN	J	996	1/1	0.08	-3.12	60,60,60,60	0
2	ZN	E	985	1/1	0.06	-3.34	70,70,70,70	0
2	ZN	J	990	1/1	0.09	-3.70	75,75,75,75	0
2	ZN	D	994	1/1	0.11	-3.95	55,55,55,55	0
2	ZN	L	992	1/1	0.04	-4.01	62,62,62,62	0
2	ZN	D	984	1/1	0.07	-4.70	63,63,63,63	0
2	ZN	B	982	1/1	0.04	-4.70	51,51,51,51	0
2	ZN	I	989	1/1	0.05	-5.29	62,62,62,62	0
2	ZN	G	987	1/1	0.06	-5.30	58,58,58,58	0
2	ZN	H	988	1/1	0.06	-5.41	60,60,60,60	0
2	ZN	A	981	1/1	0.04	-5.50	62,62,62,62	0
2	ZN	A	993	1/1	0.05	-5.64	51,51,51,51	0
2	ZN	F	986	1/1	0.07	-6.08	64,64,64,64	0
2	ZN	C	983	1/1	0.04	-7.73	67,67,67,67	0

6.5 Other polymers ⓘ

There are no such residues in this entry.