

Full wwPDB X-ray Structure Validation Report (i)

Jun 14, 2022 - 01:08 pm BST

PDB ID	:	7NE9
Title	:	A single sensor controls large variations in zinc quotas in a marine cyanobac-
		terium
Authors	:	Fulop, V.
Deposited on	:	2021-02-03
Resolution	:	2.10 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 following versions of software and data (see references (1)) were used in the production of this report:

:	4.02b-467
:	1.8.4, CSD as 541 be (2020)
:	1.13
:	FAILED
:	1.1.7 (2018)
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.28.1
	: : : : : : : :

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.10 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.



Motria	Whole archive	Similar resolution		
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
Clashscore	141614	5710 (2.10-2.10)		
Ramachandran outliers	138981	5647 (2.10-2.10)		
Sidechain outliers	138945	5648 (2.10-2.10)		

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain		
1	AAA	134	84%	5%	10%
1	BBB	134	84%	• •	10%
1	CCC	134	81%	7%	12%
1	DDD	134	82%	7% •	10%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3865 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A A A	190	Total	С	Ν	0	\mathbf{S}	0	0	0
	AAA	120	931	574	175	173	9	0		0
1	BBB	120	Total	С	Ν	0	S	0	0	0
	I DDD		931	574	175	173	9			0
1	CCC	110	Total	С	Ν	0	S	0	0	0
	118	919	566	173	171	9	0	0	0	
1 DDD	120	Total	С	Ν	0	S	0	0	0	
		931	574	175	173	9			U	

• Molecule 1 is a protein called Ferric uptake regulator family.

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	2	Total Zn 2 2	0	0
2	BBB	3	Total Zn 3 3	0	0
2	CCC	2	Total Zn 2 2	0	0
2	DDD	2	Total Zn 2 2	0	0

• Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	O 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	37	$\begin{array}{cc} \text{Total} & \text{O} \\ 37 & 37 \end{array}$	0	0
4	BBB	33	Total O 33 33	0	0
4	CCC	32	TotalO3232	0	0
4	DDD	38	$\begin{array}{cc} \text{Total} & \text{O} \\ 38 & 38 \end{array}$	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.

Note EDS failed to run properly.

• Molecule 1: Ferric uptake regulator family





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants	129.25Å 129.25 Å 77.28 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.62 - 2.10	Depositor
% Data completeness	100.0 (64.62-2.10)	Depositor
(in resolution range)	100.0 (04.02-2.10)	Depositor
R_{merge}	0.19	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.96 (at 2.10 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.194 , 0.218	Depositor
Wilson B-factor ($Å^2$)	40.3	Xtriage
Anisotropy	0.324	Xtriage
L-test for twinning ²	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
Total number of atoms	3865	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: ZN, ACT

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		
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	AAA	0.68	0/949	0.83	0/1284	
1	BBB	0.67	0/949	0.87	2/1284~(0.2%)	
1	CCC	0.68	0/936	0.86	2/1265~(0.2%)	
1	DDD	0.67	0/949	0.86	1/1284~(0.1%)	
All	All	0.68	0/3783	0.85	5/5117~(0.1%)	

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	BBB	60	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	CCC	60	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	DDD	60	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	BBB	60	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	CCC	60	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

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	AAA	931	0	893	3	0
1	BBB	931	0	893	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CCC	919	0	881	7	0
1	DDD	931	0	893	6	0
2	AAA	2	0	0	0	0
2	BBB	3	0	0	0	0
2	CCC	2	0	0	0	0
2	DDD	2	0	0	0	0
3	BBB	4	0	3	0	0
4	AAA	37	0	0	2	0
4	BBB	33	0	0	1	0
4	CCC	32	0	0	3	0
4	DDD	38	0	0	0	0
All	All	3865	0	3563	16	0

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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 2.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\hat{A})	Clash
		uistance (A)	overlap (A)
1:CCC:116:THR:HG22	4:CCC:328:HOH:O	1.58	1.03
1:AAA:61:CYS:SG	4:AAA:336:HOH:O	2.32	0.87
4:CCC:328:HOH:O	1:DDD:116:THR:HG22	1.96	0.65
1:CCC:65:PRO:HD2	4:CCC:331:HOH:O	2.02	0.59
1:CCC:124:SER:HB3	1:DDD:109:ASP:HB3	1.88	0.54
1:CCC:111:GLU:HB2	1:DDD:127:ARG:HH21	1.73	0.53
1:BBB:51:ARG:NH1	4:BBB:301:HOH:O	2.43	0.50
1:AAA:6:PRO:O	1:AAA:56:ARG:NH2	2.41	0.48
1:BBB:81:LEU:CD1	1:BBB:92:LEU:HD21	2.44	0.48
1:CCC:81:LEU:CD1	1:CCC:92:LEU:HD21	2.47	0.44
1:AAA:98:HIS:HD2	4:AAA:301:HOH:O	2.00	0.44
1:BBB:102:VAL:CG1	1:BBB:112:LEU:HD22	2.48	0.43
1:CCC:81:LEU:HD13	1:CCC:92:LEU:HD21	1.99	0.43
1:DDD:16:LEU:HD23	1:DDD:16:LEU:HA	1.91	0.43
1:CCC:111:GLU:O	1:DDD:121:GLY:HA3	2.19	0.42
1:DDD:81:LEU:CD1	1:DDD:92:LEU:HD21	2.51	0.41

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	Perce	entiles
1	AAA	116/134~(87%)	111 (96%)	5(4%)	0	100	100
1	BBB	116/134~(87%)	113~(97%)	3~(3%)	0	100	100
1	CCC	114/134~(85%)	111 (97%)	3~(3%)	0	100	100
1	DDD	116/134~(87%)	112 (97%)	3~(3%)	1 (1%)	17	12
All	All	462/536~(86%)	447 (97%)	14 (3%)	1 (0%)	47	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	103	PRO

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	AAA	101/114~(89%)	98~(97%)	3~(3%)	41 44
1	BBB	101/114 (89%)	99~(98%)	2(2%)	55 60
1	CCC	100/114~(88%)	98~(98%)	2(2%)	55 60
1	DDD	101/114 (89%)	99~(98%)	2(2%)	55 60
All	All	403/456~(88%)	394 (98%)	9 (2%)	52 57

All (9) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	AAA	55	GLN
1	AAA	102	VAL
1	AAA	127	ARG
1	BBB	24	ASP
1	BBB	102	VAL
1	CCC	75	ASP
1	CCC	102	VAL
1	DDD	24	ASP
1	DDD	127	ARG

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

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)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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	Res Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	ACT	BBB	204	-	1,3,3	5.09	1 (100%)	0,3,3	-	-



All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	204	ACT	CH3-C	5.09	1.55	1.48

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.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

