



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:32 am BST

PDB ID : 6OJC
Title : A high-resolution crystal structure of NocB thioesterase domain from No-cardicin cluster
Authors : Patel, K.D.; Gulick, A.M.
Deposited on : 2019-04-11
Resolution : 1.94 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 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 : 2.11
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) : 2.11

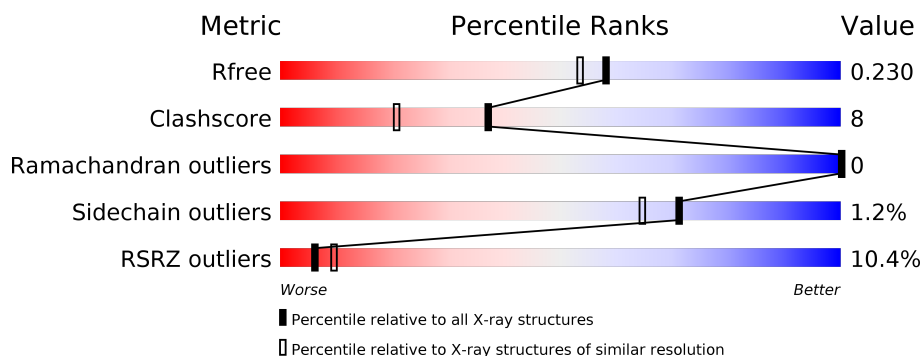
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 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 $\leq 5\%$. 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	257	<div> <div>9%</div> <div>71%</div> <div>15%</div> <div>14%</div> </div>

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	A	2007	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3337 atoms, of which 1556 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 NocB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	222	Total	C	H	N	O	S	60	1	0
			3203	1041	1549	299	311	3			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1669	MET	-	initiating methionine	UNP Q5J1Q6
A	1670	GLY	-	expression tag	UNP Q5J1Q6
A	1671	SER	-	expression tag	UNP Q5J1Q6
A	1672	SER	-	expression tag	UNP Q5J1Q6
A	1673	HIS	-	expression tag	UNP Q5J1Q6
A	1674	HIS	-	expression tag	UNP Q5J1Q6
A	1675	HIS	-	expression tag	UNP Q5J1Q6
A	1676	HIS	-	expression tag	UNP Q5J1Q6
A	1677	HIS	-	expression tag	UNP Q5J1Q6
A	1678	HIS	-	expression tag	UNP Q5J1Q6
A	1679	SER	-	expression tag	UNP Q5J1Q6
A	1680	SER	-	expression tag	UNP Q5J1Q6
A	1681	GLY	-	expression tag	UNP Q5J1Q6
A	1682	LEU	-	expression tag	UNP Q5J1Q6
A	1683	VAL	-	expression tag	UNP Q5J1Q6
A	1684	PRO	-	expression tag	UNP Q5J1Q6
A	1685	ARG	-	expression tag	UNP Q5J1Q6
A	1686	GLY	-	expression tag	UNP Q5J1Q6
A	1687	SER	-	expression tag	UNP Q5J1Q6
A	1688	HIS	-	expression tag	UNP Q5J1Q6
A	1689	MET	-	expression tag	UNP Q5J1Q6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			13	3	7	3		

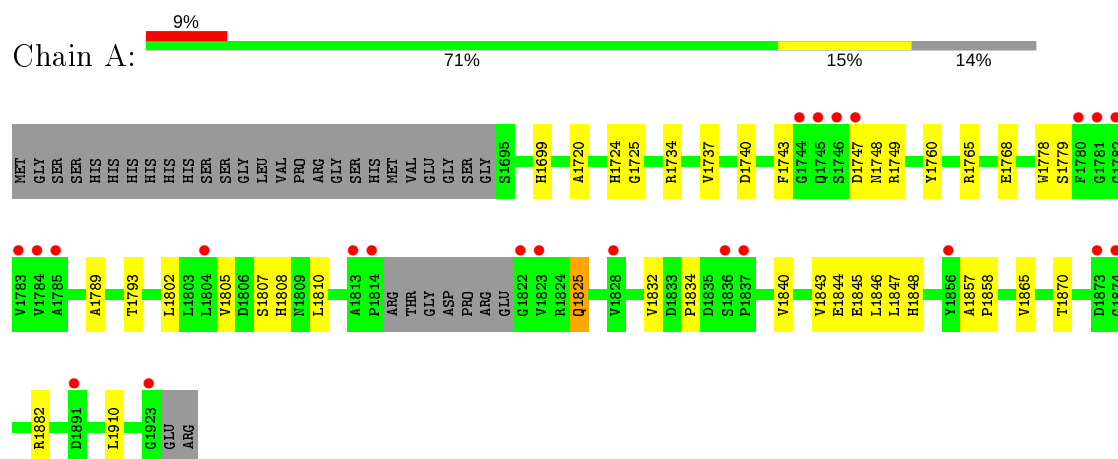
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: NocB



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.73 Å 114.73 Å 46.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.24 – 1.94 29.24 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.24-1.94) 99.8 (29.24-1.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 1.93 Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.206 , 0.230 0.207 , 0.230	Depositor DCC
R_{free} test set	1562 reflections (5.93%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3337	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	0.77	1/1698 (0.1%)	0.87	3/2326 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1760	TYR	CD1-CE1	5.21	1.47	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1765	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	A	1847	LEU	CB-CG-CD1	-5.30	101.98	111.00
1	A	1743	PHE	C-N-CA	-5.14	111.51	122.30

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	1654	1549	1582	25	0
2	A	30	0	0	0	0
3	A	6	7	8	0	0
4	A	91	0	0	4	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1781	1556	1590	25	1

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 8.

All (25) 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:1846:LEU:O	4:A:2101:HOH:O	2.15	0.64
1:A:1802:LEU:HD23	1:A:1865:VAL:HG22	1.81	0.62
1:A:1808[A]:HIS:ND1	1:A:1810:LEU:HD21	2.15	0.61
1:A:1734:ARG:NH1	1:A:1768:GLU:OE2	2.33	0.60
1:A:1740:ASP:OD2	1:A:1845:GLU:OE2	2.20	0.58
1:A:1768:GLU:HA	1:A:1768:GLU:OE1	2.05	0.56
1:A:1808[B]:HIS:CE1	1:A:1882:ARG:HG2	2.41	0.55
1:A:1843:VAL:HG23	1:A:1844:GLU:N	2.24	0.53
1:A:1840:VAL:O	1:A:1843:VAL:HG22	2.09	0.52
1:A:1808[A]:HIS:CE1	1:A:1810:LEU:HD21	2.45	0.52
1:A:1870:THR:O	4:A:2102:HOH:O	2.18	0.51
1:A:1832:VAL:O	1:A:1834:PRO:HD3	2.10	0.51
1:A:1789:ALA:O	1:A:1793:THR:HG23	2.16	0.46
1:A:1825:GLN:NE2	4:A:2106:HOH:O	2.47	0.45
1:A:1843:VAL:CG2	1:A:1844:GLU:N	2.79	0.45
1:A:1725:GLY:HA3	1:A:1910:LEU:HD21	1.99	0.45
1:A:1749:ARG:HB3	1:A:1848:HIS:CE1	2.53	0.43
1:A:1779:SER:HA	1:A:1807:SER:HA	2.01	0.43
1:A:1720:ALA:HB1	1:A:1737:VAL:HB	2.01	0.42
1:A:1778:TRP:HA	1:A:1805:VAL:HB	2.02	0.42
1:A:1857:ALA:HA	1:A:1858:PRO:HD3	1.96	0.42
1:A:1808[A]:HIS:ND1	1:A:1810:LEU:CD2	2.82	0.41
1:A:1840:VAL:HG22	1:A:1840:VAL:H	1.64	0.41
1:A:1699:HIS:HB2	4:A:2162:HOH:O	2.21	0.41
1:A:1747:ASP:O	1:A:1748:ASN:CB	2.69	0.41

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
4:A:2174:HOH:O	4:A:2174:HOH:O[5_555]	1.93	0.27

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	219/257 (85%)	214 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	166/204 (81%)	164 (99%)	2 (1%)	71	64

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

Mol	Chain	Res	Type
1	A	1724	HIS
1	A	1825	GLN

Some 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 ⓘ

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 ⓘ

7 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	2006	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	A	2002	-	4,4,4	0.13	0	6,6,6	0.41	0
2	SO4	A	2005	-	4,4,4	0.14	0	6,6,6	0.26	0
3	GOL	A	2007	-	5,5,5	1.67	1 (20%)	5,5,5	2.08	3 (60%)
2	SO4	A	2001	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	A	2003	-	4,4,4	0.17	0	6,6,6	0.35	0
2	SO4	A	2004	-	4,4,4	0.32	0	6,6,6	0.58	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	A	2007	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2007	GOL	C1-C2	2.46	1.61	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2007	GOL	O3-C3-C2	-3.29	94.43	110.20
3	A	2007	GOL	C3-C2-C1	-2.21	103.11	111.70
3	A	2007	GOL	O2-C2-C1	2.07	118.23	109.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2007	GOL	O1-C1-C2-O2
3	A	2007	GOL	O1-C1-C2-C3

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, 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	222/257 (86%)	0.65	23 (10%) 6 9	28, 52, 79, 95	10 (4%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1813	ALA	6.5
1	A	1823	VAL	6.2
1	A	1837	PRO	4.8
1	A	1874	GLY	4.5
1	A	1814	PRO	4.2
1	A	1873	ASP	4.1
1	A	1746	SER	3.6
1	A	1822	GLY	3.0
1	A	1781	GLY	2.6
1	A	1784	VAL	2.6
1	A	1782	GLY	2.6
1	A	1785	ALA	2.5
1	A	1783	VAL	2.4
1	A	1828	VAL	2.4
1	A	1923	GLY	2.4
1	A	1780	PHE	2.3
1	A	1836	SER	2.3
1	A	1856	TYR	2.2
1	A	1744	GLY	2.2
1	A	1891	ASP	2.1
1	A	1745	GLN	2.1
1	A	1804	LEU	2.1
1	A	1747	ASP	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	2004	5/5	0.49	0.31	130,133,134,137	0
2	SO4	A	2003	5/5	0.81	0.46	128,133,135,136	0
2	SO4	A	2006	5/5	0.83	0.32	125,127,132,132	0
3	GOL	A	2007	6/6	0.87	0.18	48,63,75,77	0
2	SO4	A	2005	5/5	0.88	0.35	118,121,122,125	0
2	SO4	A	2002	5/5	0.97	0.21	71,73,74,78	0
2	SO4	A	2001	5/5	0.99	0.14	72,75,77,79	5

6.5 Other polymers [i](#)

There are no such residues in this entry.