



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:02 PM GMT

PDB ID : 2DDS  
Title : Crystal structure of sphingomyelinase from *Bacillus cereus* with cobalt ion  
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Deposited on : 2006-02-02  
Resolution : 1.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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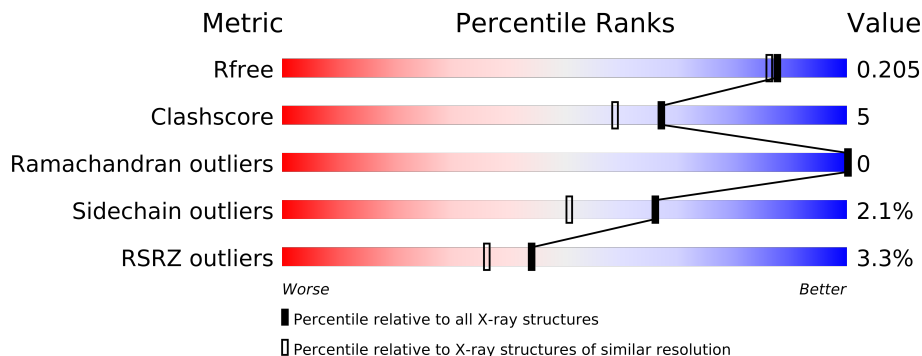
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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  $\geq 3$ , 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	306	
1	B	306	
1	C	306	
1	D	306	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CO	A	1127	-	X
2	CO	B	1125	-	X
2	CO	C	1126	-	X
2	CO	D	1128	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10448 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 Sphingomyelin phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2364	1489	395	472	8			
1	B	288	Total	C	N	O	S	0	0	0
			2289	1447	382	454	6			
1	C	298	Total	C	N	O	S	0	0	0
			2356	1485	393	470	8			
1	D	291	Total	C	N	O	S	0	0	0
			2311	1458	386	461	6			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Co	0	0
			3	3		
2	A	3	Total	Co	0	0
			3	3		
2	D	3	Total	Co	0	0
			3	3		
2	C	3	Total	Co	0	0
			3	3		

- Molecule 3 is water.

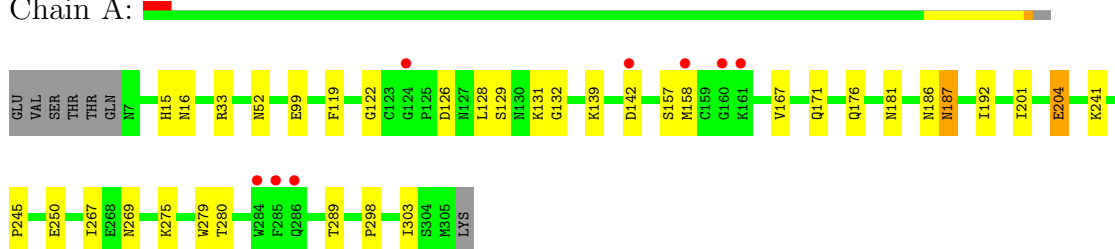
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	304	Total	O	0	0
			304	304		
3	B	261	Total	O	0	0
			261	261		
3	C	281	Total	O	0	0
			281	281		
3	D	270	Total	O	0	0
			270	270		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

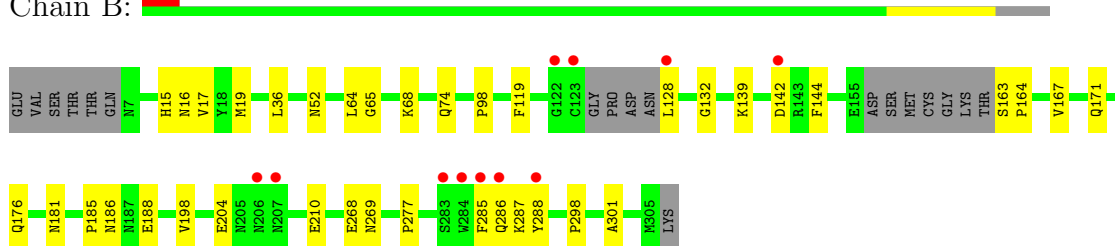
- Molecule 1: SpHINGOMYELIN phosphodiesterase

Chain A:



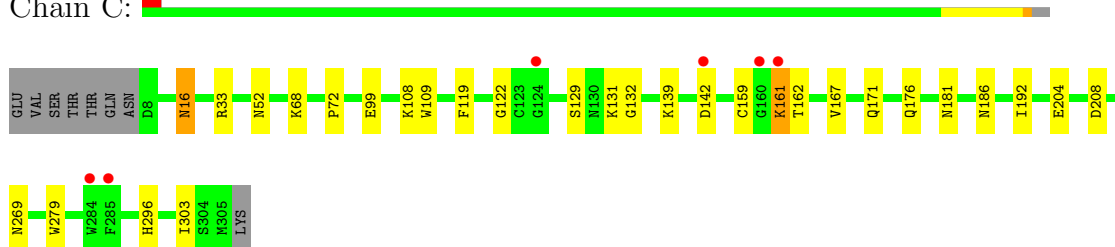
- Molecule 1: SpHINGOMYELIN phosphodiesterase

Chain B:



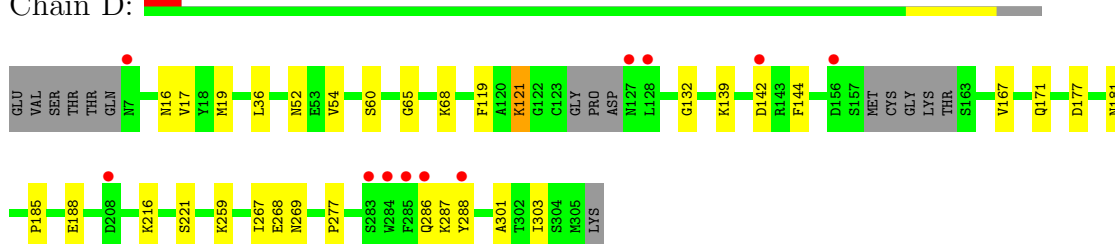
- Molecule 1: SpHINGOMYELIN phosphodiesterase

Chain C:



- Molecule 1: SpHINGOMYELIN phosphodiesterase

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.09Å 72.67Å 78.06Å 112.00° 90.05° 116.58°	Depositor
Resolution (Å)	19.67 – 1.80 35.80 – 1.77	Depositor EDS
% Data completeness (in resolution range)	91.6 (19.67-1.80) 91.0 (35.80-1.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.81 (at 1.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.202 , 0.232 0.197 , 0.205	Depositor DCC
$R_{free}$ test set	9882 reflections (10.59%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 27.2	EDS
Estimated twinning fraction	0.486 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 103230 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10448	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	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 75.13 % 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 1.3416e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities 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: CO

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	0.30	0/2421	0.59	0/3295
1	B	0.30	0/2343	0.57	0/3187
1	C	0.30	0/2413	0.59	0/3284
1	D	0.29	0/2365	0.57	0/3217
All	All	0.30	0/9542	0.58	0/12983

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	2364	0	2264	25	0
1	B	2289	0	2198	21	0
1	C	2356	0	2258	24	0
1	D	2311	0	2213	22	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	304	0	0	1	0
3	B	261	0	0	0	0
3	C	281	0	0	1	0
3	D	270	0	0	1	0
All	All	10448	0	8933	92	0

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 5.

The worst 5 of 92 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:139:LYS:HE2	1:D:142:ASP:HA	1.46	0.97
1:B:139:LYS:HE2	1:B:142:ASP:HA	1.52	0.91
1:C:139:LYS:HE2	1:C:142:ASP:HA	1.67	0.77
1:C:161:LYS:HD2	1:C:161:LYS:H	1.52	0.74
1:A:280:THR:HG22	1:A:289:THR:HG22	1.71	0.72

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	297/306 (97%)	286 (96%)	11 (4%)	0	100	100
1	B	282/306 (92%)	271 (96%)	11 (4%)	0	100	100
1	C	296/306 (97%)	286 (97%)	10 (3%)	0	100	100
1	D	285/306 (93%)	277 (97%)	8 (3%)	0	100	100
All	All	1160/1224 (95%)	1120 (97%)	40 (3%)	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	263/270 (97%)	257 (98%)	6 (2%)	63	46
1	B	254/270 (94%)	249 (98%)	5 (2%)	68	53
1	C	262/270 (97%)	255 (97%)	7 (3%)	57	39
1	D	257/270 (95%)	253 (98%)	4 (2%)	75	63
All	All	1036/1080 (96%)	1014 (98%)	22 (2%)	66	51

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	269	ASN
1	C	161	LYS
1	D	269	ASN
1	B	288	TYR
1	C	16	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	186	ASN
1	C	74	GLN
1	D	183	ASN
1	B	243	ASN
1	B	278	GLN

### 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 12 ligands modelled in this entry, 12 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	299/306 (97%)	-0.12	8 (2%) 52 44	8, 15, 34, 51	0
1	B	288/306 (94%)	-0.14	11 (3%) 38 31	8, 16, 34, 42	0
1	C	298/306 (97%)	-0.15	6 (2%) 62 56	8, 15, 34, 52	0
1	D	291/306 (95%)	-0.09	11 (3%) 38 31	9, 16, 37, 49	0
All	All	1176/1224 (96%)	-0.12	36 (3%) 44 39	8, 15, 35, 52	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	160	GLY	5.0
1	C	285	PHE	4.0
1	C	124	GLY	3.9
1	A	285	PHE	3.9
1	D	288	TYR	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

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CO	D	1128	1/1	0.23	17.02	88,88,88,88	0
2	CO	B	1125	1/1	0.23	14.49	107,107,107,107	0
2	CO	A	1127	1/1	0.15	6.04	63,63,63,63	0
2	CO	C	1126	1/1	0.20	4.06	63,63,63,63	0
2	CO	B	1122	1/1	0.07	-1.28	20,20,20,20	0
2	CO	C	1119	1/1	0.04	-1.59	21,21,21,21	0
2	CO	A	1121	1/1	0.06	-2.53	19,19,19,19	0
2	CO	A	1117	1/1	0.05	-3.89	21,21,21,21	0
2	CO	D	1124	1/1	0.03	-4.13	21,21,21,21	0
2	CO	D	1120	1/1	0.03	-5.18	20,20,20,20	0
2	CO	C	1123	1/1	0.03	-5.58	19,19,19,19	0
2	CO	B	1118	1/1	0.04	-13.08	19,19,19,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.