



wwPDB X-ray Structure Validation Summary Report ⓘ

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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 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

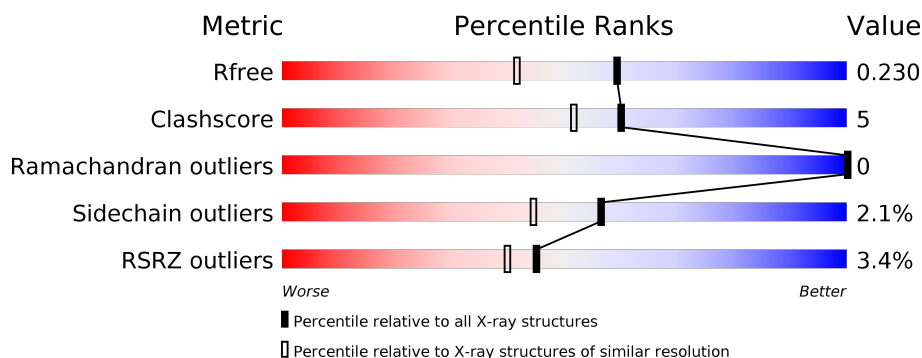
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	306	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>••</div> </div> </div>
1	B	306	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>
1	C	306	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>••</div> </div> </div>
1	D	306	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>10%</div> <div>5%</div> </div> </div>

2 Entry composition [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 1.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.232 0.199 , 0.230	Depositor DCC
R_{free} test set	9882 reflections (9.57%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.486 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10448	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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 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	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
3	A	304	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 92 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: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 [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	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 [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	263/270 (97%)	257 (98%)	6 (2%)	53 40
1	B	254/270 (94%)	249 (98%)	5 (2%)	58 47
1	C	262/270 (97%)	255 (97%)	7 (3%)	48 34
1	D	257/270 (95%)	253 (98%)	4 (2%)	65 57
All	All	1036/1080 (96%)	1014 (98%)	22 (2%)	56 44

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 [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	299/306 (97%)	-0.21	10 (3%) 46 41	8, 15, 34, 51	0
1	B	288/306 (94%)	-0.22	11 (3%) 40 35	8, 16, 34, 42	0
1	C	298/306 (97%)	-0.24	8 (2%) 54 49	8, 15, 34, 52	0
1	D	291/306 (95%)	-0.17	11 (3%) 40 35	9, 16, 37, 49	0
All	All	1176/1224 (96%)	-0.21	40 (3%) 45 40	8, 15, 35, 52	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	160	GLY	5.1
1	C	285	PHE	4.5
1	A	285	PHE	4.2
1	D	288	TYR	4.2
1	C	142	ASP	3.9

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	CO	B	1125	1/1	0.80	0.21	107,107,107,107	0
2	CO	D	1128	1/1	0.86	0.20	88,88,88,88	0
2	CO	A	1127	1/1	0.97	0.13	63,63,63,63	0
2	CO	C	1126	1/1	0.97	0.18	63,63,63,63	0
2	CO	A	1117	1/1	0.97	0.05	21,21,21,21	0
2	CO	B	1118	1/1	0.98	0.04	19,19,19,19	0
2	CO	A	1121	1/1	0.98	0.05	19,19,19,19	0
2	CO	C	1119	1/1	0.99	0.04	21,21,21,21	0
2	CO	C	1123	1/1	0.99	0.03	19,19,19,19	0
2	CO	D	1120	1/1	0.99	0.03	20,20,20,20	0
2	CO	D	1124	1/1	0.99	0.03	21,21,21,21	0
2	CO	B	1122	1/1	0.99	0.06	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.