



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:00 AM UTC

PDB ID : 2ENR / pdb_00002enr
Title : CO-CRYSTALS OF DEMETALLIZED CONCAVALIN A WITH CADMIUM HAVING A CADMIUM ION BOUND IN BOTH THE S1 SITE AND THE S2 SITE
Authors : Bouckaert, J.; Loris, R.; Wyns, L.
Deposited on : 1998-07-14
Resolution : 2.35 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

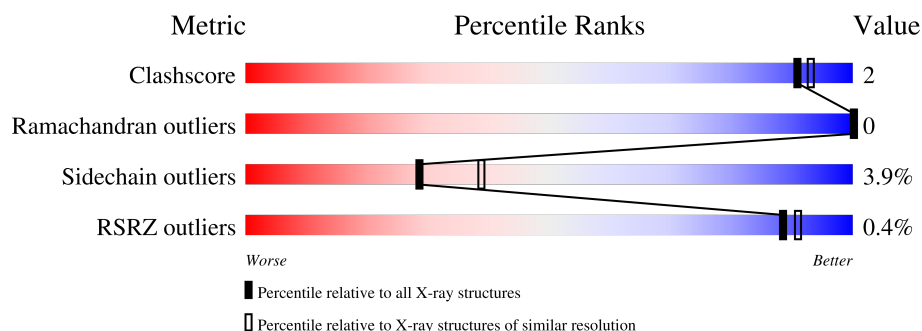
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 $\leq 5\%$. 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	237	 76% 22% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2497 atoms, of which 588 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 CONCANAVALIN A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	237	Total	C	H	N	O	S	0	0	0
			2202	1141	394	302	363	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	THR	LEU	conflict	UNP P02866
A	98	GLY	PHE	conflict	UNP P02866
A	100	TYR	PRO	conflict	UNP P02866
A	101	LYS	ILE	conflict	UNP P02866
A	102	GLU	PHE	conflict	UNP P02866
A	104	ASN	-	insertion	UNP P02866
A	105	THR	PHE	conflict	UNP P02866
A	107	LEU	THR	conflict	UNP P02866
A	108	SER	MET	conflict	UNP P02866
A	109	TRP	PHE	conflict	UNP P02866
A	110	SER	LEU	conflict	UNP P02866
A	111	PHE	MET	conflict	UNP P02866
A	112	THR	VAL	conflict	UNP P02866
A	113	SER	VAL	conflict	UNP P02866
A	114	LYS	ASN	conflict	UNP P02866
A	115	LEU	LYS	conflict	UNP P02866
A	116	LYS	VAL	conflict	UNP P02866
A	118	ASN	SER	conflict	UNP P02866
A	151	ASP	GLU	conflict	UNP P02866
A	155	GLU	ARG	conflict	UNP P02866

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cd	0	0
			2	2		

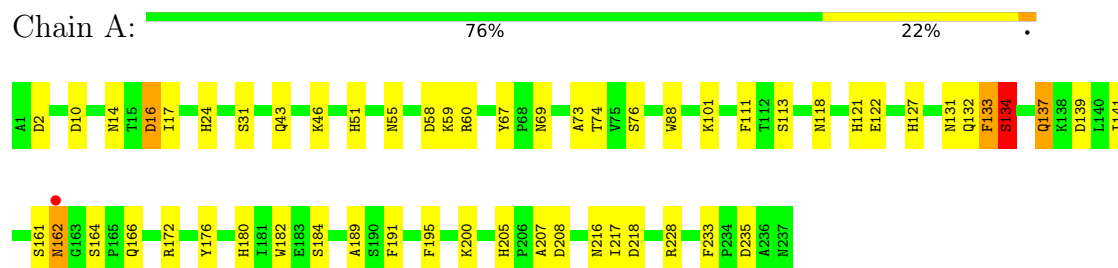
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	99	Total	H	O	0	0
			293	194	99		

3 Residue-property plots

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 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: CONCANAVALIN A



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	63.20Å 87.69Å 89.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.35 10.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.0 (10.00-2.35) 93.1 (10.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.68 (at 2.36Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.173 , (Not available) 0.163 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2497	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.01% 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: CD

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	1.17	13/1850 (0.7%)	1.90	55/2522 (2.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	PHE	CA-C	10.84	1.66	1.52
1	A	133	PHE	CB-CG	7.47	1.67	1.50
1	A	180	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	133	PHE	N-CA	-7.03	1.37	1.45
1	A	133	PHE	C-O	6.84	1.33	1.23
1	A	51	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	134	SER	CA-CB	-6.19	1.42	1.53
1	A	121	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	24	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	205	HIS	CD2-NE2	-5.66	1.31	1.37
1	A	24	HIS	CG-ND1	-5.58	1.32	1.38
1	A	10	ASP	CA-CB	-5.51	1.45	1.53
1	A	127	HIS	CD2-NE2	-5.47	1.31	1.37

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	PHE	CA-C-O	16.27	142.60	121.78
1	A	133	PHE	CA-CB-CG	14.22	128.02	113.80
1	A	133	PHE	O-C-N	-14.21	103.22	122.97
1	A	133	PHE	CD1-CG-CD2	-10.18	103.33	118.60
1	A	134	SER	CA-CB-OG	9.86	130.81	111.10
1	A	162	ASN	OD1-CG-ND2	-9.80	112.80	122.60
1	A	16	ASP	CA-CB-CG	8.60	121.20	112.60
1	A	208	ASP	N-CA-CB	-7.87	97.13	110.50
1	A	172	ARG	CB-CG-CD	-7.79	93.37	111.30
1	A	14	ASN	OD1-CG-ND2	-7.18	115.42	122.60
1	A	137	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	A	69	ASN	CA-CB-CG	7.03	119.63	112.60
1	A	217	ILE	N-CA-C	7.01	119.81	111.05
1	A	218	ASP	CA-CB-CG	6.98	119.58	112.60
1	A	131	ASN	OD1-CG-ND2	-6.86	115.75	122.60
1	A	162	ASN	CB-CG-ND2	6.75	126.53	116.40
1	A	43	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	A	207	ALA	O-C-N	-6.60	116.08	123.48
1	A	132	GLN	CA-C-O	-6.52	112.52	120.54
1	A	55	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	139	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	127	HIS	CB-CG-CD2	-6.10	123.28	131.20
1	A	14	ASN	CB-CG-ND2	6.06	125.49	116.40
1	A	162	ASN	CA-CB-CG	5.97	118.57	112.60
1	A	184	SER	N-CA-C	5.90	117.71	111.28
1	A	216	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	58	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	166	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	A	172	ARG	NE-CZ-NH2	-5.74	114.03	119.20
1	A	132	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	A	133	PHE	N-CA-CB	-5.71	102.20	110.70
1	A	235	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	59	LYS	CA-CB-CG	5.68	125.47	114.10
1	A	69	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	A	141	ILE	N-CA-C	-5.54	99.90	107.99
1	A	133	PHE	CG-CD1-CE1	5.49	130.03	120.70
1	A	164	SER	CA-C-N	5.48	125.24	119.76
1	A	164	SER	C-N-CA	5.48	125.24	119.76
1	A	2	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	88	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	A	195	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	67	TYR	N-CA-C	-5.35	100.86	109.58
1	A	69	ASN	CB-CG-ND2	5.34	124.41	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	THR	O-C-N	-5.33	117.17	123.41
1	A	191	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	73	ALA	N-CA-C	-5.28	101.27	109.72
1	A	121	HIS	CA-CB-CG	5.26	119.06	113.80
1	A	233	PHE	CA-CB-CG	-5.22	108.58	113.80
1	A	51	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	189	ALA	O-C-N	-5.21	117.10	123.30
1	A	176	TYR	N-CA-C	5.17	116.60	111.07
1	A	2	ASP	N-CA-C	5.14	116.92	110.24
1	A	216	ASN	CB-CG-ND2	5.11	124.07	116.40
1	A	127	HIS	CB-CG-ND1	5.07	130.30	122.70
1	A	182	TRP	CG-CD2-CE3	5.05	138.95	133.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	PHE	Mainchain

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	1808	394	1755	6	0
2	A	2	0	0	0	0
3	A	99	194	0	0	0
All	All	1909	588	1755	6	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 2.

All (6) 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:134:SER:HB2	1:A:137:GLN:OE1	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:HD13	1:A:228:ARG:HD3	1.92	0.51
1:A:60:ARG:HD2	1:A:76:SER:HB3	1.94	0.49
1:A:111:PHE:CE2	1:A:113:SER:HB2	2.49	0.46
1:A:16:ASP:CG	1:A:228:ARG:HH12	2.26	0.43
1:A:46:LYS:HA	1:A:46:LYS:HD3	1.96	0.42

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	235/237 (99%)	223 (95%)	12 (5%)	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	203/203 (100%)	195 (96%)	8 (4%)	28	39

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	101	LYS
1	A	118	ASN
1	A	122	GLU
1	A	134	SER
1	A	161	SER
1	A	162	ASN
1	A	200	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	41	ASN
1	A	51	HIS
1	A	69	ASN
1	A	124	ASN
1	A	131	ASN
1	A	162	ASN
1	A	237	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

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 [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	237/237 (100%)	-0.46	1 (0%) 88 91	6, 16, 38, 49	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	ASN	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 oligosaccharides 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(Å ²)	Q<0.9
2	CD	A	242	1/1	0.99	0.02	32,32,32,32	0
2	CD	A	241	1/1	1.00	0.01	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.