



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 07:01 PM EDT

PDB ID : 7AO1
Title : Crystal structure of CotB2 variant W288F in complex with alendronate
Authors : Dimos, N.; Driller, R.; Loll, B.
Deposited on : 2020-10-13
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 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

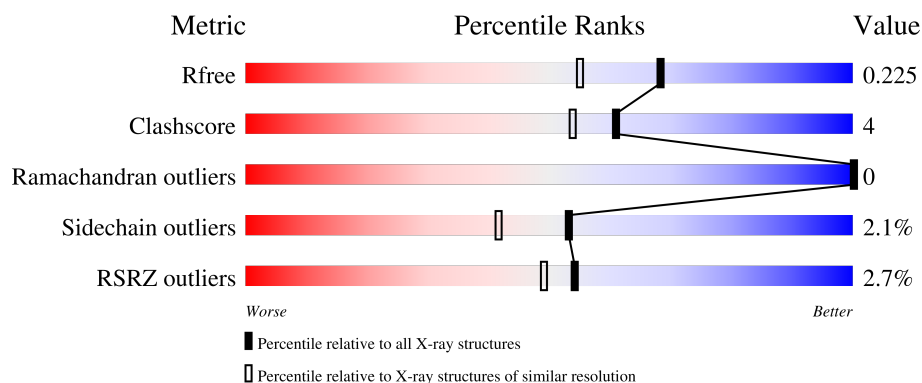
1 Overall quality at a glance

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 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	318	
1	B	318	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5457 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.

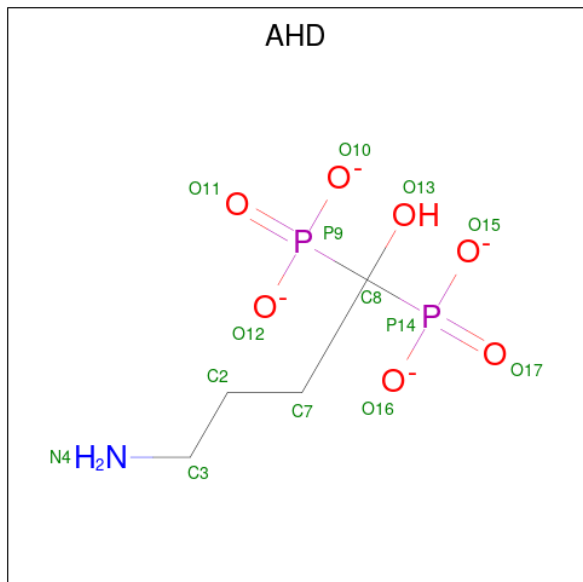
- Molecule 1 is a protein called Cyclooctat-9-en-7-ol synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	11	0
			2568	1625	440	486	17			
1	B	296	Total	C	N	O	S	0	10	0
			2503	1584	426	476	17			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	PHE	TRP	engineered mutation	UNP C9K1X5
A	308	ALA	-	expression tag	UNP C9K1X5
A	309	ALA	-	expression tag	UNP C9K1X5
A	310	ALA	-	expression tag	UNP C9K1X5
A	311	LEU	-	expression tag	UNP C9K1X5
A	312	GLU	-	expression tag	UNP C9K1X5
A	313	HIS	-	expression tag	UNP C9K1X5
A	314	HIS	-	expression tag	UNP C9K1X5
A	315	HIS	-	expression tag	UNP C9K1X5
A	316	HIS	-	expression tag	UNP C9K1X5
A	317	HIS	-	expression tag	UNP C9K1X5
A	318	HIS	-	expression tag	UNP C9K1X5
B	288	PHE	TRP	engineered mutation	UNP C9K1X5
B	308	ALA	-	expression tag	UNP C9K1X5
B	309	ALA	-	expression tag	UNP C9K1X5
B	310	ALA	-	expression tag	UNP C9K1X5
B	311	LEU	-	expression tag	UNP C9K1X5
B	312	GLU	-	expression tag	UNP C9K1X5
B	313	HIS	-	expression tag	UNP C9K1X5
B	314	HIS	-	expression tag	UNP C9K1X5
B	315	HIS	-	expression tag	UNP C9K1X5
B	316	HIS	-	expression tag	UNP C9K1X5
B	317	HIS	-	expression tag	UNP C9K1X5
B	318	HIS	-	expression tag	UNP C9K1X5

- Molecule 2 is 4-AMINO-1-HYDROXYBUTANE-1,1-DIYLDIPHOSPHONATE (three-letter code: AHD) (formula: $C_4H_9NO_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			14	4	1	7	2		
2	B	1	Total	C	N	O	P	0	0
			14	4	1	7	2		

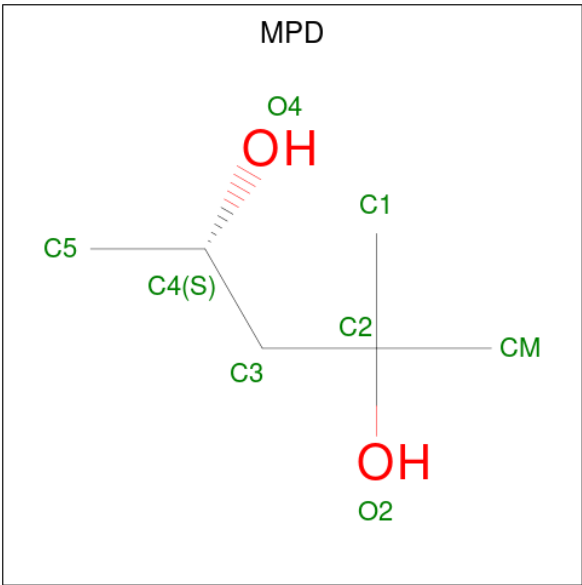
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Mg	0	0
			3	3		
3	B	3	Total	Mg	0	0
			3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	184	Total	O	0	22
			184	184		
6	B	142	Total	O	0	8
			142	142		

- Molecule 1: Cyclooctat-9-en-7-ol synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.67Å 57.10Å 57.35Å 91.05° 116.31° 102.01°	Depositor
Resolution (Å)	20.45 – 1.80 46.68 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.1 (20.45-1.80) 89.1 (46.68-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.173 , 0.226 0.173 , 0.225	Depositor DCC
R_{free} test set	2100 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5457	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, CL, AHD, MG

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	0.68	0/2632	0.73	1/3564 (0.0%)
1	B	0.64	0/2560	0.70	0/3468
All	All	0.66	0/5192	0.72	1/7032 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	LEU	CA-CB-CG	5.05	126.92	115.30

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	A	2568	0	2458	20	0
1	B	2503	0	2399	28	0
2	A	14	0	9	0	0
2	B	14	0	9	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	14	1	0
5	B	16	0	28	1	0
6	A	184	0	0	2	0
6	B	142	0	0	0	0
All	All	5457	0	4917	45	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 4.

The worst 5 of 45 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:186:TRP:CE3	5:A:406:MPD:H13	2.26	0.70
1:A:314:HIS:NE2	6:A:501:HOH:O	2.25	0.68
1:B:112:MET:HE1	1:B:117:HIS:HD2	1.62	0.65
1:B:111:ASP:O	1:B:305:ARG:HD3	1.99	0.62
1:A:24:GLU:OE1	1:A:27:ARG:NH2	2.36	0.58

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	311/318 (98%)	307 (99%)	4 (1%)	0	100	100
1	B	304/318 (96%)	297 (98%)	7 (2%)	0	100	100
All	All	615/636 (97%)	604 (98%)	11 (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	281/281 (100%)	277 (99%)	4 (1%)	67	59
1	B	274/281 (98%)	267 (97%)	7 (3%)	46	32
All	All	555/562 (99%)	544 (98%)	11 (2%)	53	44

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	271	ASP
1	B	275	GLN
1	B	304	SER
1	B	283	TYR
1	B	86	SER

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 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AHD	B	401	3	13,13,13	1.41	2 (15%)	19,21,21	2.65	8 (42%)
5	MPD	B	407	-	7,7,7	0.51	0	9,10,10	1.24	1 (11%)
5	MPD	B	406	-	7,7,7	0.71	0	9,10,10	1.42	1 (11%)
2	AHD	A	401	3	13,13,13	1.45	3 (23%)	19,21,21	1.73	4 (21%)
5	MPD	A	406	-	7,7,7	0.53	0	9,10,10	0.97	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
2	AHD	B	401	3	-	6/23/23/23	-
5	MPD	B	407	-	-	4/5/5/5	-
5	MPD	B	406	-	-	0/5/5/5	-
2	AHD	A	401	3	-	1/23/23/23	-
5	MPD	A	406	-	-	0/5/5/5	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	AHD	O13-C8	-3.29	1.40	1.44
2	A	401	AHD	P9-C8	2.85	1.87	1.85
2	B	401	AHD	P9-C8	-2.69	1.83	1.85
2	A	401	AHD	P14-O16	-2.36	1.48	1.54
2	A	401	AHD	O13-C8	-2.31	1.41	1.44

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	AHD	C2-C7-C8	-7.14	103.62	116.02
2	A	401	AHD	C2-C7-C8	-4.73	107.80	116.02
2	B	401	AHD	O10-P9-C8	4.44	115.97	106.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	AHD	O16-P14-O15	3.80	118.95	108.24
2	B	401	AHD	P14-C8-P9	-3.51	106.43	112.72

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	407	MPD	C1-C2-C3-C4
5	B	407	MPD	O2-C2-C3-C4
5	B	407	MPD	C2-C3-C4-C5
2	B	401	AHD	C2-C7-C8-P9
2	B	401	AHD	C2-C7-C8-P14

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	407	MPD	1	0
5	A	406	MPD	1	0

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	302/318 (94%)	-0.21	6 (1%) 65 61	15, 28, 47, 84	0
1	B	296/318 (93%)	-0.02	10 (3%) 45 39	19, 31, 56, 91	0
All	All	598/636 (94%)	-0.12	16 (2%) 54 49	15, 30, 55, 91	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	ALA	6.9
1	B	301	ASP	5.4
1	A	315	HIS	5.4
1	A	314	HIS	4.9
1	B	298	ALA	4.1

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 monosaccharides 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
5	MPD	B	406	8/8	0.91	0.15	18,33,44,45	0
5	MPD	B	407	8/8	0.91	0.13	37,42,48,52	0
5	MPD	A	406	8/8	0.93	0.12	31,38,42,46	0
3	MG	B	404	1/1	0.97	0.05	32,32,32,32	0
2	AHD	B	401	14/14	0.98	0.08	25,29,39,43	0
2	AHD	A	401	14/14	0.98	0.09	21,23,30,45	0
4	CL	B	405	1/1	0.98	0.07	34,34,34,34	0
3	MG	A	402	1/1	0.99	0.05	27,27,27,27	0
4	CL	A	405	1/1	0.99	0.07	28,28,28,28	0
3	MG	A	403	1/1	0.99	0.04	23,23,23,23	0
3	MG	A	404	1/1	0.99	0.03	23,23,23,23	0
3	MG	B	402	1/1	0.99	0.07	32,32,32,32	0
3	MG	B	403	1/1	0.99	0.04	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.