



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 02:23 am BST

PDB ID : 2V4A
Title : Crystal structure of the SeMet-labeled prolyl-4 hydroxylase (P4H) type I from green algae *Chlamydomonas reinhardtii*.
Authors : Koski, M.K.; Hieta, R.; Bollner, C.; Kivirikko, K.I.; Myllyharju, J.; Wierenga, R.K.
Deposited on : 2007-06-28
Resolution : 1.93 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
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

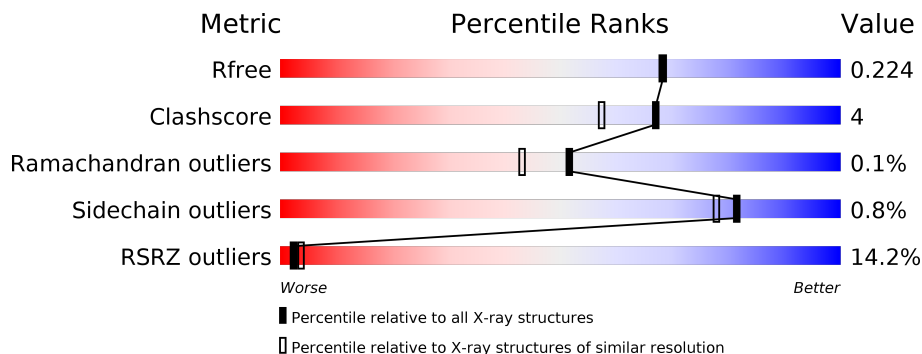
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	233	 7% 73% 5% 22%
1	B	233	 7% 72% 5% 25%
1	C	233	 13% 75% 5% 20%
1	D	233	 16% 68% 14% 17%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6127 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 PROLYL-4 HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	182	1423	906	243	265	3	6	0	0	0
1	B	174	1359	868	232	250	3	6	0	0	0
1	C	187	1461	931	250	271	3	6	0	0	0
1	D	194	1530	976	259	286	3	6	0	0	0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

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



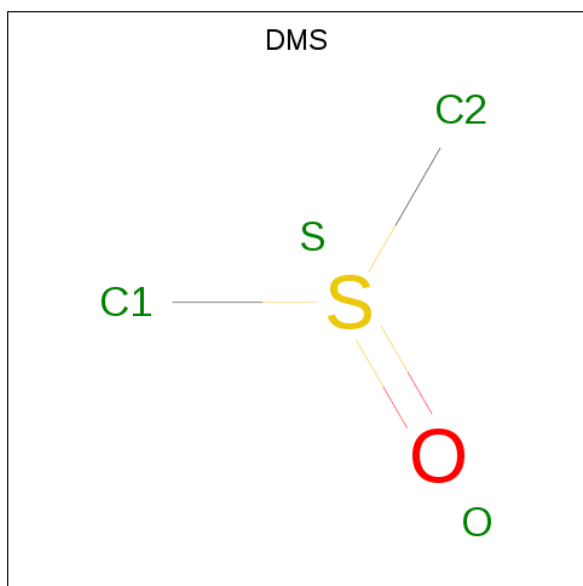
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

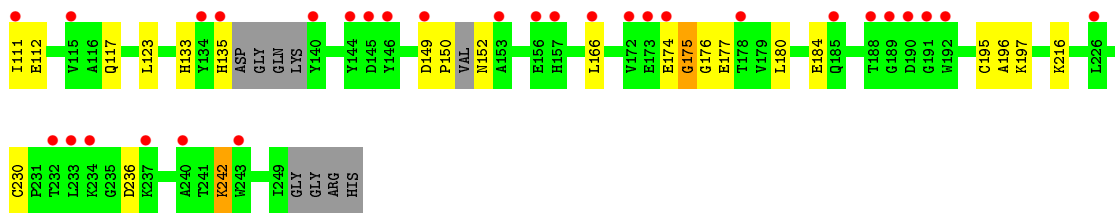
- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	99	Total O 99 99	0	0
6	B	88	Total O 88 88	0	0
6	C	67	Total O 67 67	0	0
6	D	59	Total O 59 59	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.49Å 137.49Å 88.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 1.93 19.86 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.87-1.93) 99.6 (19.86-1.93)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.93Å)	Xtrriage
Refinement program	REFMAC 5.3.0028	Depositor
R, R_{free}	0.188 , 0.223 0.191 , 0.224	Depositor DCC
R_{free} test set	3176 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtrriage
Anisotropy	0.230	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6127	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GOL, DMS, SO4, CL

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	0.83	0/1451	0.75	2/1951 (0.1%)
1	B	0.94	2/1386 (0.1%)	0.78	1/1864 (0.1%)
1	C	0.80	2/1490 (0.1%)	0.68	1/2004 (0.0%)
1	D	0.87	5/1566 (0.3%)	0.76	3/2110 (0.1%)
All	All	0.86	9/5893 (0.2%)	0.74	7/7929 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	32	GLY	C-O	19.94	1.55	1.23
1	C	194	GLU	CD-OE2	10.82	1.37	1.25
1	B	32	GLY	CA-C	10.28	1.68	1.51
1	C	194	GLU	CD-OE1	10.26	1.36	1.25
1	D	236	ASP	CG-OD2	9.36	1.46	1.25

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	32	GLY	CA-C-O	-11.46	99.98	120.60
1	D	236	ASP	CB-CG-OD1	-10.24	109.08	118.30
1	D	135	HIS	CA-CB-CG	-6.04	103.32	113.60
1	C	34	LEU	CA-CB-CG	5.59	128.15	115.30
1	D	236	ASP	CB-CG-OD2	5.33	123.10	118.30

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	1423	0	1402	7	0
1	B	1359	0	1345	3	0
1	C	1461	0	1446	7	0
1	D	1530	0	1473	27	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	2	0
3	D	6	0	8	0	0
4	A	5	0	0	0	0
5	B	8	0	12	0	0
6	A	99	0	0	2	0
6	B	88	0	0	1	0
6	C	67	0	0	0	0
6	D	59	0	0	4	0
All	All	6127	0	5710	44	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 4.

The worst 5 of 44 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:74:MSE:HE3	1:D:96:THR:HB	1.47	0.96
1:D:39:ARG:HH11	1:D:39:ARG:CG	1.85	0.89
1:C:50:ARG:HH11	3:C:1251:GOL:H11	1.39	0.87
1:D:195:CYS:HG	1:D:230:CYS:HG	0.89	0.83
1:D:39:ARG:HH11	1:D:39:ARG:HG2	1.48	0.77

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)
1:D:150:PRO:CB	1:D:150:PRO:CB[8_554]	2.03	0.17

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	174/233 (75%)	171 (98%)	3 (2%)	0	100	100
1	B	166/233 (71%)	166 (100%)	0	0	100	100
1	C	179/233 (77%)	174 (97%)	5 (3%)	0	100	100
1	D	184/233 (79%)	178 (97%)	5 (3%)	1 (0%)	29	17
All	All	703/932 (75%)	689 (98%)	13 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	175	GLY

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	154/192 (80%)	152 (99%)	2 (1%)	69	62
1	B	147/192 (77%)	147 (100%)	0	100	100
1	C	158/192 (82%)	158 (100%)	0	100	100
1	D	164/192 (85%)	161 (98%)	3 (2%)	59	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	623/768 (81%)	618 (99%)	5 (1%)	81	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	THR
1	A	185	GLN
1	D	39	ARG
1	D	166	LEU
1	D	242	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	B	185	GLN
1	D	117	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 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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
3	GOL	C	1251	-	5,5,5	0.37	0	5,5,5	0.36	0
3	GOL	A	1251	-	5,5,5	0.29	0	5,5,5	0.89	0
5	DMS	B	1252	-	3,3,3	2.65	1 (33%)	3,3,3	0.76	0
3	GOL	B	1251	-	5,5,5	0.40	0	5,5,5	0.27	0
3	GOL	D	1251	-	5,5,5	0.40	0	5,5,5	0.47	0
4	SO4	A	1252	-	4,4,4	0.23	0	6,6,6	0.42	0
5	DMS	B	1253	-	3,3,3	2.67	1 (33%)	3,3,3	0.55	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	C	1251	-	-	4/4/4/4	-
3	GOL	A	1251	-	-	4/4/4/4	-
3	GOL	D	1251	-	-	0/4/4/4	-
3	GOL	B	1251	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1253	DMS	O-S	4.46	1.80	1.50
5	B	1252	DMS	O-S	4.42	1.80	1.50

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1251	GOL	O1-C1-C2-C3
3	B	1251	GOL	O1-C1-C2-C3
3	B	1251	GOL	C1-C2-C3-O3
3	B	1251	GOL	O2-C2-C3-O3
3	C	1251	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1251	GOL	2	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	176/233 (75%)	0.61	16 (9%) 9 14	20, 26, 31, 43	0
1	B	168/233 (72%)	0.63	16 (9%) 8 12	21, 26, 31, 35	0
1	C	181/233 (77%)	0.99	31 (17%) 1 2	20, 26, 31, 37	0
1	D	188/233 (80%)	1.07	38 (20%) 1 1	11, 26, 31, 34	0
All	All	713/932 (76%)	0.83	101 (14%) 2 4	11, 26, 31, 43	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	HIS	7.1
1	C	94	THR	6.5
1	A	36	GLU	5.9
1	D	153	ALA	5.9
1	D	140	TYR	5.7

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
3	GOL	A	1251	6/6	0.79	0.20	49,50,51,52	0
3	GOL	B	1251	6/6	0.80	0.20	55,56,57,57	0
5	DMS	B	1252	4/4	0.84	0.28	57,58,58,59	0
3	GOL	C	1251	6/6	0.88	0.15	45,47,48,48	0
3	GOL	D	1251	6/6	0.88	0.12	54,56,57,58	0
5	DMS	B	1253	4/4	0.93	0.17	68,69,69,69	0
2	CL	D	1250	1/1	0.98	0.09	45,45,45,45	0
4	SO4	A	1252	5/5	0.98	0.14	31,32,35,36	0
2	CL	C	1250	1/1	0.98	0.13	35,35,35,35	0
2	CL	B	1250	1/1	0.99	0.15	28,28,28,28	0
2	CL	A	1250	1/1	0.99	0.11	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.