



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1OXW / pdb_00001oxw
Title : The Crystal Structure of SeMet Patatin
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Deposited on : 2003-04-03
Resolution : 2.20 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

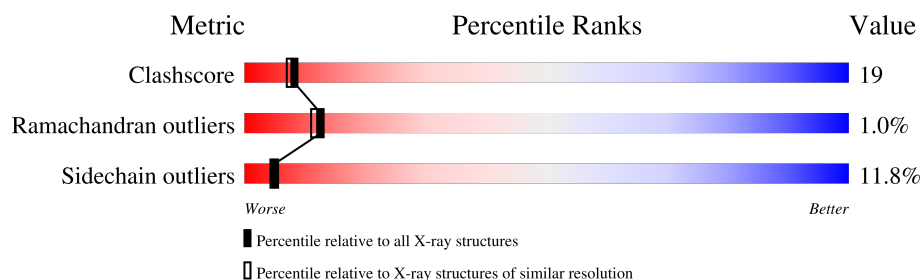
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	
1	C	373	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8871 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 Patatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	Se	0	0	0
			2787	1769	454	553	11			
1	B	359	Total	C	N	O	Se	0	0	0
			2782	1765	453	553	11			
1	C	362	Total	C	N	O	Se	0	0	0
			2804	1779	457	556	12			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MSE	-	expression tag	UNP Q8LPW4
A	15	HIS	-	expression tag	UNP Q8LPW4
A	16	HIS	-	expression tag	UNP Q8LPW4
A	17	HIS	-	expression tag	UNP Q8LPW4
A	18	HIS	-	expression tag	UNP Q8LPW4
A	19	HIS	-	expression tag	UNP Q8LPW4
A	20	HIS	-	expression tag	UNP Q8LPW4
A	21	ALA	-	expression tag	UNP Q8LPW4
A	22	MSE	-	expression tag	UNP Q8LPW4
A	28	MSE	MET	modified residue	UNP Q8LPW4
A	58	MSE	MET	modified residue	UNP Q8LPW4
A	85	MSE	MET	modified residue	UNP Q8LPW4
A	131	MSE	MET	modified residue	UNP Q8LPW4
A	180	MSE	MET	modified residue	UNP Q8LPW4
A	253	MSE	MET	modified residue	UNP Q8LPW4
A	284	MSE	MET	modified residue	UNP Q8LPW4
A	290	MSE	MET	modified residue	UNP Q8LPW4
A	298	MSE	MET	modified residue	UNP Q8LPW4
A	331	MSE	MET	modified residue	UNP Q8LPW4
A	339	MSE	MET	modified residue	UNP Q8LPW4
B	1014	MSE	-	expression tag	UNP Q8LPW4
B	1015	HIS	-	expression tag	UNP Q8LPW4
B	1016	HIS	-	expression tag	UNP Q8LPW4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1017	HIS	-	expression tag	UNP Q8LPW4
B	1018	HIS	-	expression tag	UNP Q8LPW4
B	1019	HIS	-	expression tag	UNP Q8LPW4
B	1020	HIS	-	expression tag	UNP Q8LPW4
B	1021	ALA	-	expression tag	UNP Q8LPW4
B	1022	MSE	-	expression tag	UNP Q8LPW4
B	1028	MSE	MET	modified residue	UNP Q8LPW4
B	1058	MSE	MET	modified residue	UNP Q8LPW4
B	1085	MSE	MET	modified residue	UNP Q8LPW4
B	1131	MSE	MET	modified residue	UNP Q8LPW4
B	1180	MSE	MET	modified residue	UNP Q8LPW4
B	1253	MSE	MET	modified residue	UNP Q8LPW4
B	1284	MSE	MET	modified residue	UNP Q8LPW4
B	1290	MSE	MET	modified residue	UNP Q8LPW4
B	1298	MSE	MET	modified residue	UNP Q8LPW4
B	1331	MSE	MET	modified residue	UNP Q8LPW4
B	1339	MSE	MET	modified residue	UNP Q8LPW4
C	2014	MSE	-	expression tag	UNP Q8LPW4
C	2015	HIS	-	expression tag	UNP Q8LPW4
C	2016	HIS	-	expression tag	UNP Q8LPW4
C	2017	HIS	-	expression tag	UNP Q8LPW4
C	2018	HIS	-	expression tag	UNP Q8LPW4
C	2019	HIS	-	expression tag	UNP Q8LPW4
C	2020	HIS	-	expression tag	UNP Q8LPW4
C	2021	ALA	-	expression tag	UNP Q8LPW4
C	2022	MSE	-	expression tag	UNP Q8LPW4
C	2028	MSE	MET	modified residue	UNP Q8LPW4
C	2058	MSE	MET	modified residue	UNP Q8LPW4
C	2085	MSE	MET	modified residue	UNP Q8LPW4
C	2131	MSE	MET	modified residue	UNP Q8LPW4
C	2180	MSE	MET	modified residue	UNP Q8LPW4
C	2253	MSE	MET	modified residue	UNP Q8LPW4
C	2284	MSE	MET	modified residue	UNP Q8LPW4
C	2290	MSE	MET	modified residue	UNP Q8LPW4
C	2298	MSE	MET	modified residue	UNP Q8LPW4
C	2331	MSE	MET	modified residue	UNP Q8LPW4
C	2339	MSE	MET	modified residue	UNP Q8LPW4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	156	Total O 156 156	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	169	Total 169	O 169	0	0
2	C	173	Total 173	O 173	0	0

V2345	T2229	Q2112	MSE
G2346	Q2237	Q2122	HIS
E2347	K2238	Y2129	HIS
L2350	A2243	V2133	HIS
K2351	S2244	L2134	HIS
K2352	T2245	Q2135	HIS
P2353	R2246	E2136	ALA
N2358	Y2250	K2137	M2022
T2361	K2251	L2138	A2023
E2364	K2252	T2141	Q2024
K2367	M2253	R2142	L2025
R2380	T2260	Q2145	M2028
K2383	G2261	T2148	G2036
ALA	E2265	D2156	G2037
SER	T2269	I2157	G2038
TYR	Y2270	K2158	T2039
	E2274	T2166	R2040
	H2282	K2167	G2041
	L2285	S2168	L2042
	V2286	N2169	E2049
	M2290	S2173	L2048
	Q2308	P2174	Q2054
	A2309	E2175	M2058
	L2310	D2182	D2059
	Q2320	Y2185	N2060
	E2321	A2190	R2065
	L2324	P2195	F2070
	T2327	P2196	S2077
	T2328	H2197	T2078
	T2329	T2201	L2081
	E2330	N2202	L2082
	N2331	T2203	T2088
	D2332	S2204	P2089
	D2333	N2205	N2090
	E2336	G2206	E2091
	A2337	D2207	N2092
	N2338	E2208	N2093
	M2339	Y2209	R2094
	E2340	N2212	P2095
	L2341	L2213	K2100
	L2342	V2214	E2101
	V2343	D2215	T2102
	Q2344	T2220	V2103
			P2104
			F2105
			Y2106
			F2107
			E2108

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.18Å 171.42Å 129.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.220 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8871	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.58	3/2830 (0.1%)	0.95	12/3825 (0.3%)
1	B	0.57	1/2825 (0.0%)	0.94	12/3819 (0.3%)
1	C	0.55	0/2847	0.92	10/3847 (0.3%)
All	All	0.56	4/8502 (0.0%)	0.94	34/11491 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1290	MSE	SE-CE	-6.17	1.76	1.95
1	A	298	MSE	SE-CE	-5.55	1.78	1.95
1	A	339	MSE	SE-CE	-5.13	1.80	1.95
1	A	290	MSE	SE-CE	-5.11	1.80	1.95

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	TYR	N-CA-C	7.40	120.41	109.24
1	A	213	LEU	N-CA-C	7.05	121.16	109.95
1	B	1270	TYR	N-CA-C	7.03	119.85	109.24
1	C	2213	LEU	N-CA-C	6.97	121.03	109.95
1	B	1102	ILE	N-CA-C	6.94	117.05	110.53

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	2787	0	2756	109	0
1	B	2782	0	2746	111	0
1	C	2804	0	2773	104	0
2	A	156	0	0	2	0
2	B	169	0	0	3	0
2	C	173	0	0	5	0
All	All	8871	0	8275	321	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 19.

The worst 5 of 321 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:B:1201:THR:HG22	1:B:1209:TYR:HB3	1.41	0.98
1:C:2201:THR:HG22	1:C:2209:TYR:HB3	1.46	0.97
1:C:2261:GLY:H	1:C:2320:GLN:HE22	1.11	0.96
1:A:201:THR:HG22	1:A:209:TYR:HB3	1.46	0.96
1:B:1261:GLY:H	1:B:1320:GLN:HE22	1.14	0.95

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	358/373 (96%)	337 (94%)	15 (4%)	6 (2%)	7	5
1	B	357/373 (96%)	335 (94%)	19 (5%)	3 (1%)	16	16
1	C	360/373 (96%)	340 (94%)	18 (5%)	2 (1%)	21	23
All	All	1075/1119 (96%)	1012 (94%)	52 (5%)	11 (1%)	12	11

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	SER
1	A	358	ASN
1	B	1244	SER
1	B	1356	GLU
1	C	2244	SER

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	302/300 (101%)	264 (87%)	38 (13%)	4	4
1	B	302/300 (101%)	265 (88%)	37 (12%)	4	4
1	C	304/300 (101%)	272 (90%)	32 (10%)	6	6
All	All	908/900 (101%)	801 (88%)	107 (12%)	5	5

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1244	SER
1	B	1373	LEU
1	C	2328	THR
1	B	1253	MSE
1	B	1350	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2212	ASN
1	C	2320	GLN
1	C	2358	ASN
1	B	1024	GLN
1	A	382	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](#)

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.