



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 04:50 pm BST

PDB ID : 1OXW
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 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

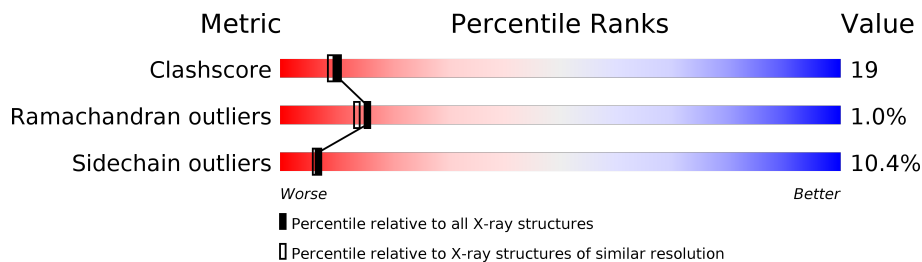
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	373	65% 25% 5% . .
1	B	373	68% 23% 5% . .
1	C	373	68% 25% . .

2 Entry composition [i](#)

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
			Total	C	N	O	Se			
1	A	360	2787	1769	454	553	11	0	0	0
1	B	359	2782	1765	453	553	11	0	0	0
1	C	362	2804	1779	457	556	12	0	0	0

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

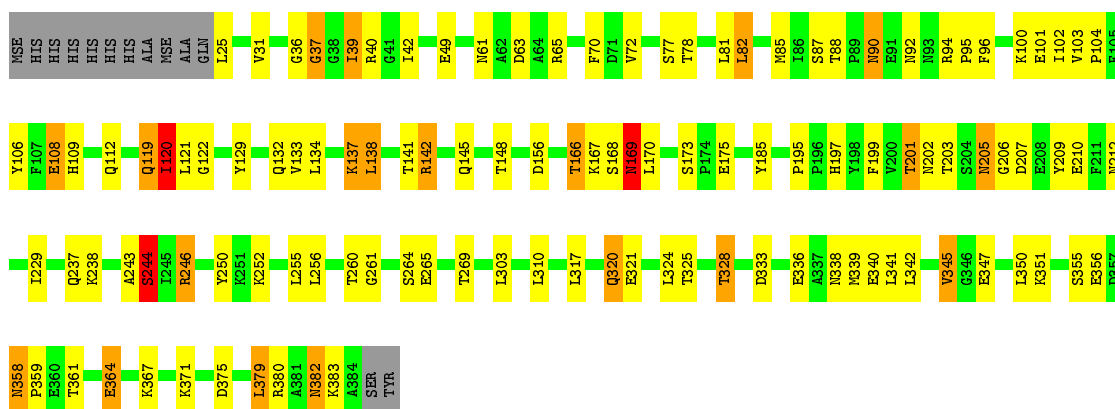
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

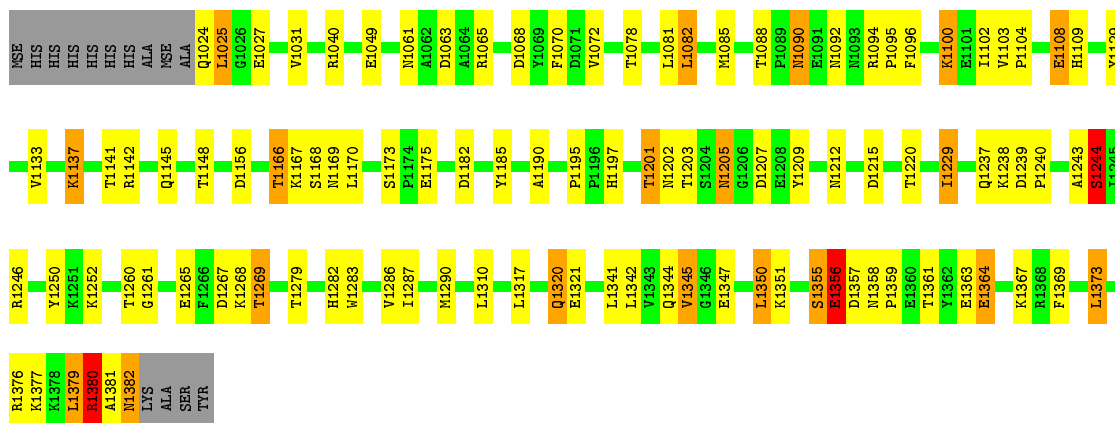
- Molecule 1: Patatin

Chain A: 



- Molecule 1: Patatin

Chain B: 



- Molecule 1: Patatin

Chain C: 

A2243	Y2129	MSE	K2100
S2244	V2133	HIS	E2101
T2245	L2134	HIS	I2102
R2246	L2135	HIS	V2103
Y2250	Q2135	HIS	P2104
K2251	E2136	HIS	F2105
K2252	K2137	HIS	Y2106
M2253	L2138	ALA	F2107
L2254	T2141	A2023	E2108
T2260	R2142	Q2024	Q2112
G2261	R2145	L2025	
E2265	T2148	M2028	
T2269	D2156	G2036	
E2274	T2157	G2037	
H2282	K2158	G2038	
L2285	T2166	T2039	
V2286	K2167	R2040	
M2290	S2168	G2041	
Q2308	M2169	I2042	
A2309	S2173	L2048	
L2310	E2175	E2049	
Q2320	D2182	Q2054	
E2321	Y2185	M2058	
L2324	A2190	R2065	
T2327	P2195	F2070	
T2328	E2196	S2077	
T2329	H2197	T2078	
M2331	V2200	L2081	
D2332	T2201	L2082	
E2336	M2202	T2088	
A2337	T2203	P2089	
M2338	S2204	M2090	
M2339	M2205	E2091	
E2340	G2206	M2092	
L2341	D2207	M2093	
L2342	E2208	R2094	
V2343	Y2209	P2095	
Q2344	M2212	K2100	
Y2345	D2215	E2101	
E2347	D2215	I2102	
L2350	T2220	V2103	
K2351	Q2237	P2104	
P2353	K2238	F2105	
		Y2106	
		F2107	
		E2108	
		Q2112	
D2357			
M2358			
T2361			
E2364			
R2380			
K2383			
ALA			
SER			
THR			

4 Data and refinement statistics

Xtrriage (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.	Xtrriage
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	0.45	0/2830	0.64	0/3825
1	B	0.44	0/2825	0.63	0/3819
1	C	0.44	0/2847	0.63	0/3847
All	All	0.45	0/8502	0.63	0/11491

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	2787	0	2756	106	0
1	B	2782	0	2746	105	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	312	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 312 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%)	9	6
1	B	357/373 (96%)	335 (94%)	19 (5%)	3 (1%)	19	19
1	C	360/373 (96%)	340 (94%)	18 (5%)	2 (1%)	25	26
All	All	1075/1119 (96%)	1012 (94%)	52 (5%)	11 (1%)	15	14

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 [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	302/300 (101%)	265 (88%)	37 (12%)	4	4
1	B	302/300 (101%)	271 (90%)	31 (10%)	7	6
1	C	304/300 (101%)	278 (91%)	26 (9%)	10	10
All	All	908/900 (101%)	814 (90%)	94 (10%)	7	6

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1100	LYS
1	B	1252	LYS
1	C	2320	GLN
1	B	1108	GLU
1	B	1201	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1197	HIS
1	B	1320	GLN
1	C	2338	ASN
1	B	1205	ASN
1	B	1338	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 carbohydrates 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.