



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 27, 2024 – 06:58 PM EDT

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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

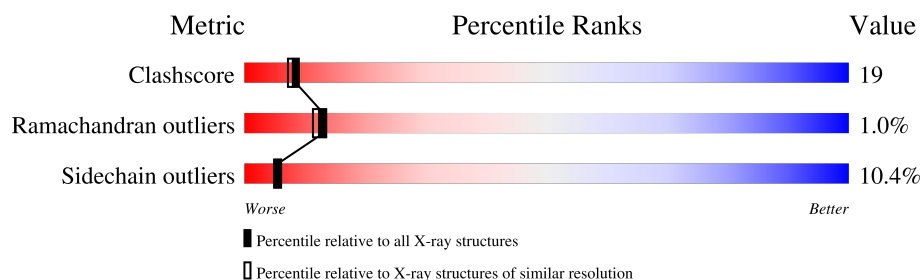
1 Overall quality at a glance

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	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (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

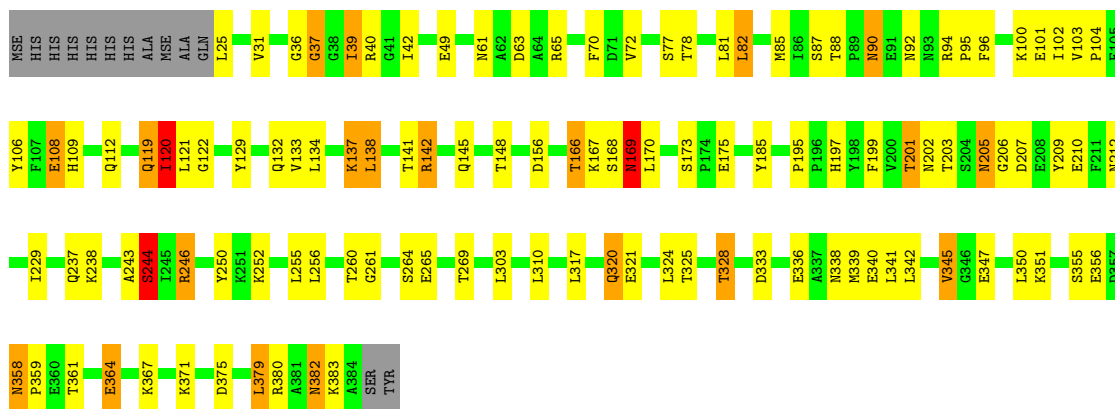
3 Residue-property plots

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. 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.

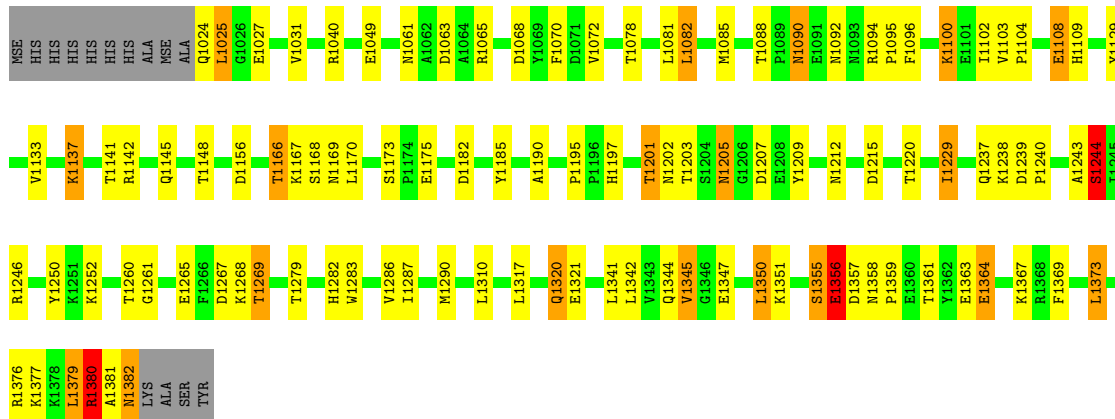
• Molecule 1: Patatin

Chain A: 



• Molecule 1: Patatin

Chain B: 



• Molecule 1: Patatin

Chain C: 

Y2129	A2243	D2357	HSE
V2133	S2244	N2358	HIS
L2134	T2245	T2361	HIS
Q2135	R2246	T2364	HIS
E2136	Y2250	E2364	HIS
K2137	K2251	R2380	HIS
L2138	K2252	K2383	ALA
T2141	M2253	ALA	M2022
R2142	L2254	SER	A2023
Q2145	T2260	TYR	Q2024
T2148	G2261		L2025
D2156	E2265		M2028
T2157	T2269		G2036
K2158	E2274		G2037
T2166	H2282		G2038
K2167	L2285		T2039
S2168	V2286		R2040
N2169	M2290		G2041
S2173	Q2308		T2042
P2174	A2309		L2048
E2175	L2310		E2049
D2182	Q2320		Q2054
Y2185	E2321		M2058
A2190	L2324		R2065
P2195	T2327		F2070
P2196	T2328		S2077
H2197	T2329		T2078
V2200	E2330		L2081
T2201	M2331		L2082
N2202	D2332		T2088
T2203	E2336		P2089
S2204	A2337		N2090
N2205	N2338		F2091
G2206	M2339		N2092
D2207	E2340		N2093
E2208	L2341		R2094
Y2209	L2342		P2095
N2212	V2343		K2100
D2215	Q2344		E2101
T2220	V2345		I2102
Q2237	G2346		P2103
K2238	E2347		P2104
P2353	L2350		Y2105
	K2351		Y2106
	K2352		F2107
			E2108
			Q2112

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

5.1 Standard geometry

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

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%)	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%)	22	23
All	All	1075/1119 (96%)	1012 (94%)	52 (5%)	11 (1%)	13	12

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	3
1	B	302/300 (101%)	271 (90%)	31 (10%)	6	5
1	C	304/300 (101%)	278 (91%)	26 (9%)	8	9
All	All	908/900 (101%)	814 (90%)	94 (10%)	5	5

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

Mol	Chain	Res	Type
1	B	1345	VAL
1	C	2100	LYS
1	B	1351	LYS
1	B	1379	LEU
1	C	2138	LEU

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

Mol	Chain	Res	Type
1	C	2145	GLN
1	C	2382	ASN
1	C	2197	HIS
1	C	2320	GLN
1	B	1090	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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.