wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 04:50 pm BST

PDB ID	:	1OXW
Title	:	The Crystal Structure of SeMet Patatin
Authors	:	Rydel, T.J.; Williams, J.M.; Krieger, E.; Moshiri, F.; Stallings, W.C.; Brown, S.M.; Pershing, J.C.; Purcell, J.P.; Alibhai, M.F.
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

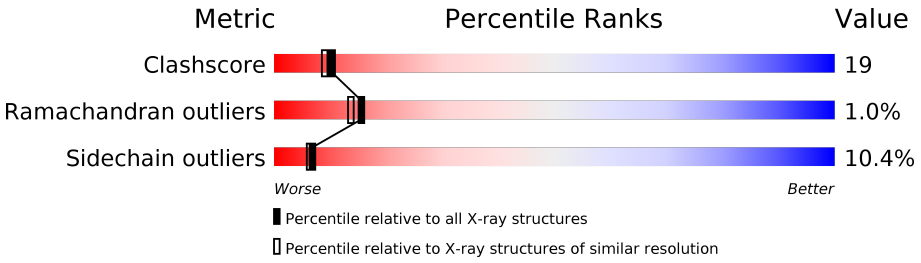
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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 <=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

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 O 169 169	0	0
2	C	173	Total O 173 173	0	0

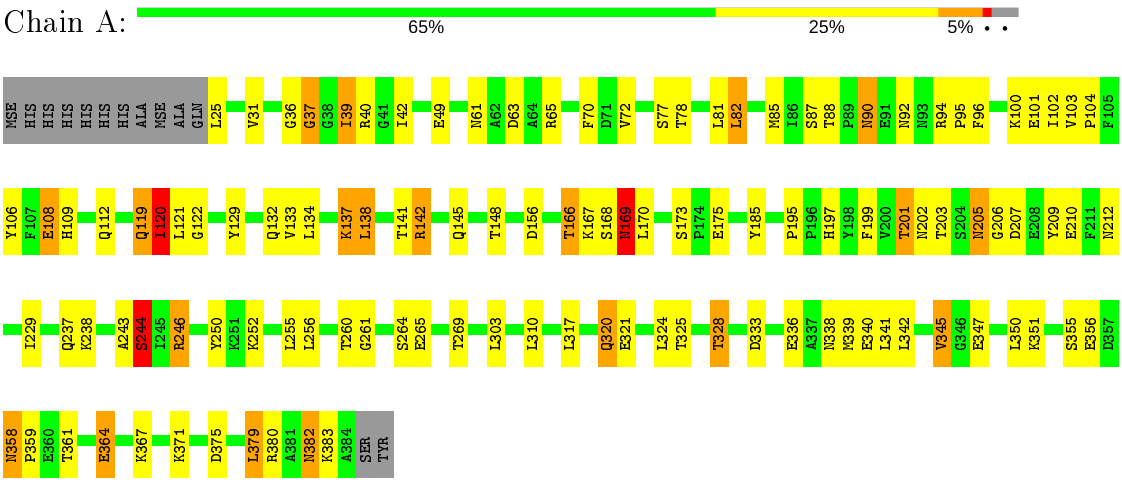
3 Residue-property plots (i)

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.

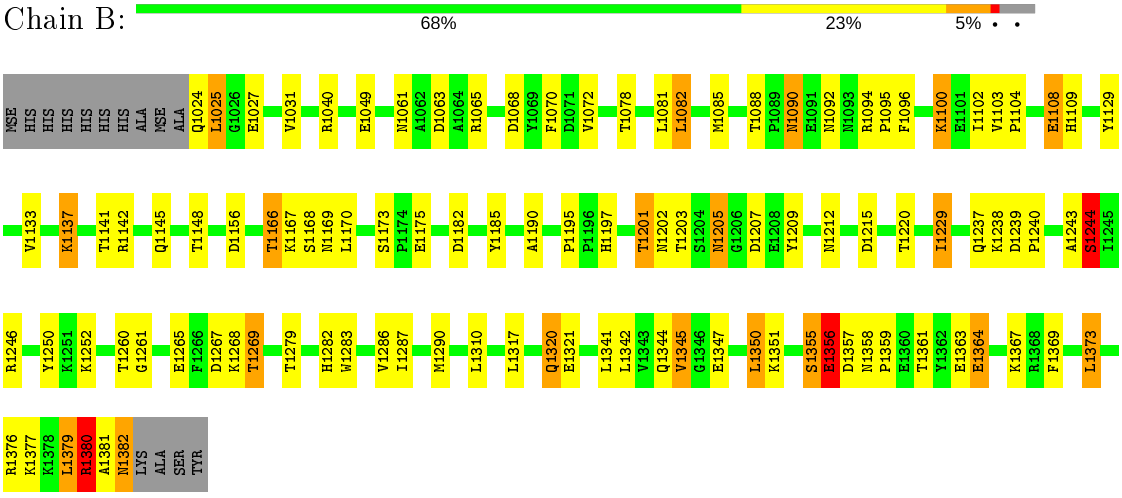
- Molecule 1: Patatin

Chain A:



- Molecule 1: Patatin

Chain B:



- Molecule 1: Patatin

Chain C:


MSE HIS HIS HIS HIS HIS HIS ALA M2022 A2023 Q2024 L2025 M2028 G2036 G2037 G2038 I2039 R2040 G2041 I2042 L2048 E2049 Q2054 M2058 R2065 F2070 S2077 T2078 L2081 L2082 T2088 P2089 N2090 E2091 N2092 N2093 R2094 P2095 K2100 E2101 I2102 V2103 P2104 F2105 Y2106 F2107 E2108 Q2112
Y2129 V2133 L2134 Q2135 E2136 K2137 L2138 T2141 R2142 Q2145 T2148 D2156 I2157 K2158 T2166 K2167 S2168 N2169 S2173 P2174 E2175 D2182 Y2185 A2190 P2195 P2196 H2197 V2200 T2201 N2202 T2203 S2204 N2205 G2206 D2207 E2208 Y2209 N2212 D2215 T2220 Q2237 K2238
A2243 S2244 I2245 R2246 Y2250 K2251 K2252 N2253 L2254 T2260 G2261 E2265 T2269 E2274 H2282 L2285 V2286 M2290 Q2308 A2309 L2310 Q2320 E2321 L2324 T2327 T2328 T2329 E2330 M2331 D2332 E2336 A2337 N2338 M2339 E2340 L2341 L2342 V2343 Q2344 V2345 G2346 E2347 L2350 K2351 K2352 P2353
D2357 N2358 T2361 E2364 R2380 K2383 ALA SER TYR

4 Data and refinement statistics (i)

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%)	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.